SOME STUDIES IN ONE SPEED NEUTRON TRANSPORT THEORY

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CERTIFICATE

Certified that this work entitled, 'Some Studies in One Speed Neutron Transport Theory', has been done by Mr. Keshab Gangopadhyay under my supervision and has not been submitted elsewhere for a degree.

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SYNOPSIS

The present thesis is divided in four chapters. Chapters II and III describe the major contribution of the present work.

Chapter I extensively reviews the work done during the last two decades in P_N-approximation and application of Case's theory in standard neutron transport problems. In the light of the review, it tries to establish the objective of the present work.

Chapter II develops the formulation of Transport theoretic P_N approximation (TP_N). The methodology is based on the framework of conventional P_N-approximation in conjunction with Case's exact treatment of the one-speed neutron transport equation. Firstly, it demonstrates that the use of all the roots of conventional P_N approximation is not mathematically justified and the exact asymptotic decay constant ν_o must be used in place of its P_N counterpart in describing the asymptotic flux. Formal solution of the transport equation is then constructed with the asymptotic part being of the same nature as exact solution and the transient part terminated as in conventional P_N approximation. The second part of the scheme generalizes the Marshak's free-surface boundary condition. This is achieved by introduction of a parameter α_N in the first equation of the set of Marshak boundary conditions. α_N is evaluated by forcing the asymptotic flux for the source-free Milne problem to be identically same as the exact transport theory asymptotic flux. The Milne problem is chosen as a reference problem as it leads to the free surface conditions. The same α_N can be used for any other one-speed transport problem involving a free surface. Analytical expressions for the parameter α_N for TP_1 and TP_3 approximations are presented. While analytical expressions for α_N can be similarly constructed for higher order approximations, a simple formula is prescribed for evaluating α_N $(N > 3)$ to avoid prohibitively-increasing algebraic complexity. The formalism is then applied to different standard transport problems - the emergent distribution and leakage for the Milne problem, the scalar flux in Milne problem when $c = 1$, the leakage in constant source Milne problem and the critical problem. The calculation shows that both the emergent distribution and the leakage for the source-free Milne problem improve significantly in the TP_N approximation. As a check on the justification of the present scheme for the special case of $c = 1$, the scalar flux obtained by this scheme for Milne problem is compared with the exact and P_N values. TP_1 flux is superior to P_1 flux for large values of x, while TP_3 improves P_3 calculation for all x except for very small values of x. Constant source Milne problem and the criticality problem are next considered where, unlike the source-free Milne problem, α_N is explicitly used in the formulation. In the constant source Milne problem it is found that TP_N method worsens the P_N leakage value for low values of c. The reason for the failure of TP_N method in this case may be attributed to poor transient flux representation and also to the fact that extrapolation distance for constant source problem for small values of c is widely different from that of source-free Milne problem. As is apparent from calculation, TP_N significantly improves the critical slab thickness. TP_1 gives the end-point result and TP_3 improves the result further. TP_N theory is then applied to modify the interface conditions and a typical fuel-moderator cell problem is then analyzed. It is found that TP_N-approximation significantly improves the disadvantage factor compared to its P_N counterpart. Finally it is concluded that the present scheme usually leads to improved results except in cases where the transient component is overwhelmingly predominant. Also, unlike asymptotic diffusion theory, any order of approximation can be systematically constructed in this method.

Chapter III poses the finite slab problem in a multiplying medium as an inverse eigenvalue problem and treats it functional analytically to establish the existence of the critical thickness. Numerical estimate of critical thickness is also obtained by functional analytic methods. The set of two coupled Fredholm equations as obtained in Case's theory for a finite slab problem with an incident beam on one of the surfaces is combined together to form a single Fredholm integral equation. Critical slab problem is defined by putting the non-homogeneous term equal to zero. The equation is then recast in a simpler form for mathematical analysis. This is analyzed as a general eigenvalue equation in which an operator $\mathbb{K}(b)$ depends on a parameter b. The problem we are interested in is that one which specifies the eigenvalue and determines the parameter b (i.e. the operator). Hence it is called the inverse eigenvalue problem. The operator $\mathbb{K}(b)$ is completely continuous in $\mathbb{L}_2$ except for those b where the kernel has singularity. By straight-forward application of Gohberg theorem in the range of analyticity of the operator-valued function $\mathbb{K}(b)$, the existence of critical thickness is proved. Analyticity criterion on $\mathbb{K}(b)$ shows that the critical thickness b_c must be less than the end-point result. This fact is not reflected by P_N calculation. The kernel $K(\nu , \nu', b)$ of the integral equation (ν, $\nu' \varepsilon (0,1)$ are dependent variables of the integral equation) is then analyzed for positivity in ν, ν' for all b. Restriction on positivity is necessary for elegant application of bounds on spectral radius of linear operators. It is established that an approximate problem which slightly departs from the original equation (numerical calculation substantiates this) satisfies the positivity criterion. In the general problem, $\lambda(b) = 1$ defines the critical slab problem and our intention is to solve the equation $\lambda(b) = 1$

for critical half-thickness b_c. Estimates of spectral radius in its simplest form are used to find the critical thickness. Considering the crudity of the bounds of spectral radius, the result is found to be fairly accurate. No sophistication in calculational technique has been attempted to improve the result further. This is because that the present work is not meant for the calculation of critical thickness but is aimed at precise formulation of a class of inverse eigenvalue problems. Numerical calculation is only done as a check on the hypothesis adapted in the proposed analysis. The choice of the critical problem is only incidental and the theory can be applied to the general class of similar problems. At the end of the chapter, a discussion on the existence of solution for a slab albedo problem is given.

In the last chapter, a separate Transport-theoretic P_N-approximation scheme has been constructed for constant source type problems. It has been shown that the escape probability results for a finite slab containing uniform source are significantly improved in the present method over conventional P_N-approximation, whereas TP_N-formalism based on source-free Milne problem fails absolutely in this case for low values of c. A discussion on possible further extension of the present work is also given.

CHAPTER I

INTRODUCTION

The phenomenon of neutron transport, which is of primary significance in the analysis and design of nuclear reactors, is adequately described by the linear Boltzmann equation. In the most general form of the Boltzmann equation, the neutron angular density appears as a function of space, angle, energy and time. Unfortunately this equation in its entire generality is not solvable analytically in most cases. Thus, one has to consider the problem in a restricted subspace with drastic simplifying assumptions so as to be able to treat neutron diffusion theoretically. The present thesis restricts the analysis to one speed neutron transport in slab geometry. In this approximation, the neutron speed is assumed to be unchanged in a collision though angular deflection occurs. The assumption may seem to be severe to describe the physics of neutron transport but it is well-known that 'the mathematical analyst is no respector of physics if he sees a chance to obtain an exact solution'.[1] Nevertheless, one-speed theory has great importance for various reasons. Firstly, analytical closed-form solutions can be obtained for different standard problems. These solutions provide a thorough mathematical understanding of the Boltzmann equation and is exceedingly useful as a qualitative guide for practical reactor calculations. The standard problems also provide a sample set for testing computer codes. The more important factor is that the solution of one-speed equation forms the basis of multigroup approximation, frequently used in the design of nuclear reactors.

The framework of the present thesis is based on exact and approximate methods of solving one-speed neutron transport equation. For exact treatment, we choose Case's singular eigenfunction expansion technique while spherical harmonics method is our choice for approximate analysis. A great deal of work has been done on Case's singular eigenfunction method and the technique has become almost standard, in preference to the older Wiener-Hopf technique in the exact treatment of neutron transport. From the point of view of analysis, the P_N-approximation is possibly the most popular approximate method of one-speed transport equation solution. As is well-known, the P_N-approximation tends to exact solution as $N \to \infty$, and the objective behind improvements in P_N-approximation is only to achieve faster convergence i.e., more accurate solution with a lower order of approximation.

During last two decades, much effort has been made to improve the P_N-approximation by incorporating transport-theoretic effects in it. However, in these works better angular flux representation through modification of usual boundary conditions in a general way did not receive proper attention.

The present work is broadly divided into two parts. In Chapter II, a Transport-theoretic P_N-approximation scheme has been formulated for the approximate solution of one-speed equation. The asymptotic part of the solution has an exact angular flux representation while the transient is still in the framework of P_N-approximation. Numerical calculations of different standard transport problems have been performed. Through a better angular flux representation, faster convergence of solution is achieved. In Chapter III, the critical and slab albedo problem have been analyzed by using Case's method and function analytical theorems. The critical problem is studied as an inverse eigenvalue problem of a Fredholm integral equation. Numerical calculation of critical thickness has also been performed by function analytical methods. The results are good considering the simplicity of the method which does not involve the actual solution of governing Fredholm equations.

1.1 Literature Review:

The literature review on exact solution of one-speed transport equation is given first to enable a better understanding of approximate methods in the light of exact analysis.

Among the early works in the exact treatment of one-speed transport equation, the first noteworthy technique was developed by Wiener and Hopf [2]. In this method, a functional equation is obtained by suitable Fourier or Laplace transform of the original one-speed equation and this equation is then solved by the method of complex analysis. The method was first successfully applied for the solution of Milne problem in the case of radiative heat transfer and then for different boundary value problems of neutron transport theory. However, with the advent of Case's work [3] on singular eigenfunctions, the Wiener-Hopf method lost its supremacy. The idea of singular eigenfunction expansion technique was first put forward by Davison [4] and then elegantly developed with proper mathematical sophistication by Case. The basic idea of the method is to separate the space and angle variables by assuming the angular flux $\psi(x, \mu)$ of the form $\psi(x, \mu) = e^{-x/\nu} \phi_\nu(\mu)$ and then to construct a complete set of eigenmodes in a suitably chosen function space. It is demonstrated that the spectrum of ν is a set of two discrete eigenvalues $\pm\nu_0$ outside the interval (-1, 1) and a continuous part $\nu \varepsilon (-1,1)$. The formal solution of the transport equation is then constructed as

$$\psi(x, \mu) = a_{0+} \cdot e^{-x/\nu_0} \phi_{0+}(\mu) + a_{0-} e^{x/\nu_0} \phi_{0-}(\mu)$$

$$+ \int_{-1}^{1} A(\nu) e^{-x/\nu} \phi_\nu(\mu) d\nu$$

where $\phi_{0\pm}(\mu)$, $\phi_\nu(\mu)$ are the eigenfunctions corresponding to discrete and continuous spectra of ν respectively. $a_{0\pm}$ and $A(\nu)$ are the expansion coefficients which are to be determined from source or boundary conditions. For a full-range problem, this condition is of the form

$$f(\mu) = a_{0+} \phi_{0+}(\mu) + a_{0-} \phi_{0-}(\mu) + \int_{-1}^{1} A(\nu) \phi_\nu(\mu) d\nu$$

The full-range completeness theorem proves that the functions $\phi_{0\pm}(\mu)$ and $\phi_\nu(\mu)$ are complete for a given function $f(\mu)$ defined on the full range of $\mu \varepsilon (-1, 1)$ and determines the expansion coefficients by orthogonality relations.[5] For a more realistic problem consisting of a half-space only, the boundary condition takes the general form

$$f(\mu) = a_{0+} \phi_{0+}(\mu) + \int_{0}^{1} A(\nu) \phi_\nu(\mu) d\nu \qquad 0 \leq \mu \leq 1$$

The expansion function $f(\mu)$ defines a particular problem as for example, $f(\mu)$ is $\delta(\mu - \mu_o)$ for half-space albedo problem and $-\phi_{o-}(\mu)$ in the Milne problem. It can be shown by half range completeness theorem that the functions $\phi_{o+}(\mu)$ and $\phi_\nu(\mu)$, $0 \leq \nu \leq 1$ are complete for the expansion function $f(\mu)$ defined on the range $0 \leq \mu \leq 1$. The expansion coefficients are determined by application of the associated orthogonality relations [5]. This basic methodology of Case's work is discussed elaborately in the texts of Case and Zweifel [5] and Bell and Glasstone [6]. Applications of Case's method are given in reference [5] and a review article by McCormick and Kuŝĉer entitled 'Singular eigenfunction expansion technique' [7]. Case's formalism for isotropic scattering is extended to the case of anisotropic scattering by Mika [8]. Mendelson and Summerfield [9] applied the singular function method to problems involving two adjacent half-spaces. They succeeded in establishing suitable orthogonality relations similar to those obtained for a single medium. The completeness of eigenfunctions for multigroup neutron transport was taken up by various workers [10-14]. Numerical calculations on multigroup transport problems were done by Pahor and Shultis [10], Siewert and Ishiguro [11], Metcalf and Zweifel [12]. The computations, in general, are much involved and it is doubtful that singular eigenfunction expansion method can be elegantly applied for worthwhile numerical calculations.

The discussion presented in the earlier section is based on either infinite medium or half-space problems. As the present work is concerned with the finite slab, we emphasize this particular problem. In his formulation, Mitsis [15] considered a finite slab of half-thickness b in a multiplying medium (i.e., c, number of secondaries per primary, greater than 1) and derived a singular integral equation in terms of the expansion coefficients using the symmetry and boundary conditions of the problem. The singular integral equation was then transformed to a set of two coupled Fredholm integral equations by standard methods [16]. The solution of the problem is given by the following equation with $a_{0+} = a_{0-} = 1$, say,

$$\begin{aligned}\psi(x, \mu) &= \psi_{0+}(x, \mu) + \psi_{0-}(x, \mu) \\ &\quad + \int_{-1}^{1} A(\nu)\, \psi_{\nu}(x, \mu)\, d\nu\end{aligned}$$

$A(\nu)$ obeys the following Fredholm integral equations

$$\begin{aligned}e^{b/\mu} A(\mu) &= -e^{b/\nu_0} [\phi_{0+}(\mu) X(\nu_0) + \phi_{0-}(\mu) X(-\nu_0) e^{-2b/\nu_0}] \\ &\quad x (\nu_0^2 - \mu^2).(1-c) X(-\mu) g(c,\mu) - (\nu_0^2 - \mu^2)(1-c) \\ &\quad x\, g(c,\mu) X(-\mu) \int_0^1 \frac{(c/2)\nu X(-\nu) A(\nu) e^{-b/\nu}}{(\nu + \mu)} d\nu\end{aligned} \tag{1.1}$$

$$\nu_o e^{b/\nu_o} [X(\nu_o) - e^{-2b/\nu_o} X(-\nu_o)] = \int_0^1 A(\nu) e^{-b/\nu} \nu X(-\nu) d\nu \qquad (1.2)$$

where, $X(\nu)$ is the well-known X-function of Case's theory and $g(c, \mu)$ is given by

$$g(c, \mu) = \frac{1}{(1 - c\mu \tanh^{-1}\mu)^2 + \frac{c^2\pi^2\mu^2}{4}}$$

Equation (1.2) is the exact criticality relation - a relation between the material concentration (c or ν_o) and the thickness (2b) of the slab. Thus $A(\nu)$ has to obey the Fredholm equation (1.1) and at the same time satisfy the criticality condition (1.2). Mitsis constructed Neumann series solution for equations (1.1) and (1.2). However, because of the complexity of the nature of equations, the iterations could not be extended beyond first order approximation (which itself is rather complicated). The equation (1.1) is written in the form

$$A(\nu) = A_1(\nu) + \lambda \int_0^1 K(\nu, \alpha) A(\alpha) d\alpha$$

the Neumann series solution of which is given by

$$A(\nu) = A_1(\nu) + \lambda \int_0^1 K(\nu, \alpha) A_1(\alpha) d\alpha + \lambda^2 \int_0^1\int_0^1 K(\nu, \alpha) K(\alpha, \beta) A_1(\beta) d\alpha\, d\beta + \ldots \qquad (1.3)$$

For a zero-th order or diffusion-like approximation where there is no transient component, Mitsis assumed $A\ \ (\nu) = 0$. The criticality condition in this case can be reduced to the familiar 'end-point result' [5].

$$b_c = b_{\text{end-point}} = \frac{\pi}{2} |\nu_o| - Z_o$$

The corresponding solution is exactly of the same form as diffusion theory except the use of transport theory ν_o in place of P_1 asymptotic decay constant. In the first-order approximation, $A\cdot(\nu)$ in equation (1.3) was set equal to the inhomogeneous term $A_1\ (\nu)$ and the corresponding solution was obtained after fairly lengthy calculations. Although, in principle, the scheme is applicable for higher order approximations, no such attempt was made by Mitsis, because of the complicated nature of functions involved. It is to be noted, however, that the Neumann series converges rapidly except for systems with dimensions less than one mean free path i.e. for large c. Thus, for critical thickness calculation the first order or even the zero-th order approximation is fairly accurate for all practical purposes. In studying the slab albedo problem, McCormick and Mendelson [17] followed an approach similar to that of Mitsis and constructed a slightly different iterative scheme for the solution of the coupled Fredholm equationsbased on Neumann series expansion. The Albedo problem transforms to the criticality problem in the absence of incident neutrons and the results obtained by McCormik and Mendelson are same as Mitsis's. The conservative convergence criterion for Neumann series that the modulus of eigenvalue be greater than the spectral radius of the operator, puts a restriction on the validity of solution for the Fredholm equations. Thus the integral equations are not solvable by Neumann series expansion for a certain range of parameters although the solution actually exists in those cases. Both Leonard and Mullikin [18] and Bowden et al [19] apply a similar approach to construct Neumann series solutions for their integral equations. Erdmann [20] gives an elaborate discussion on different approximation schemes for Neumann series solution of the coupled integral equations that arise in the case of neutron transport problems in finite media. In none of the works mentioned sofar, the integral equations were actually solved - zero-th order or at best first order approximations could only be constructed.

Among the approximate methods, the spherical harmonics approximation is simple and popular as an analytical tool, whereas the discrete angle approximation is more suited for numerical work. A good account of these methods are compiled in reference [6]. We concentrate on P_N-approximation only as it is of relevance to the present work. The detailed analysis of P_N-approximation can be found in two classical papers by Marshak [21] and Mark [22], and the two widely-used free surface boundary conditions in this approximate method go by their name. The basic idea of the method is to expand the neutron angular flux in a series of Legendre polynomial and replace the transport equation by an infinite set of coupled differential equations in terms of the moments of angular neutron density. In P_N approximation, the infinite set is truncated to a finite set of (N+1) equations by imposing the somewhat arbitrary condition that the derivative of (N+1)-th moment of the angular flux vanishes. Because of this truncation, the continuous spectrum $\nu \varepsilon (-1, 1)$ is replaced by (N - 1) discrete values and thus the eigen-value spectrum is purely discrete. A major short coming of conventional P_N-approximation is that for small values of c and N not too large, all the (N + 1) eigenvalues lie in (-1, 1) while it is known that the largest $|\nu_j|$ corresponding to the asymptotic flux is greater than 1. The error involved in this approximation is mainly due to the truncation of infinite number of differential equations to a finite set and also due to the fact that exact boundary condition cannot be satisfied in such an approximation. Eversince the P_N approximation was proposed for neutron transport calculation, much effort has been made towards its improvement. The first such attempt was on the P_1 or classical diffusion approximation. This improved theory, called the asymptotic diffusion theory, is described by Case, de Hoffmann and Placzek [23] and by Davison [4]. In this theory, the diffusion coefficient of P_1 approximation is replaced by $(1-c)\ \nu^2/\Sigma$ on an adhoc basis. Although the exponential growth or decay of neutrons flux is accurately described by this theory, the stringent boundary condition of continuity of scalar flux at an interface leads to wrong flux amplitude deep within the medium. Pomraning and Clark [24] developed a slightly different asymptotic diffusion theory based on variational methods that gives exact transport growth or decay and also predicts the flux amplitude correctly. This was done by allowing a flux discontinuity at an interface. Selengut [25] also used variational methods to introduce the asymptotic diffusions theory where it is found that both current and scalar flux are discontinuous at an interface. Pomraning [26] later developed another asymptotic diffusion theory to incorporate the advantages of both the earlier methods of Pomraning and Clark [24] and Selengut [25]. In his asymptotic theory, the scalar flux is allowed to be discontinuous by introduction of two parameters $\beta(c)$ and $\Gamma(c)$. These parameters are evaluated by normalizing the formalism to two standard reference half-space problem solutions. A supplementary separate diffusion-like theory is proposed for transient flux. Unlike the asymptotic flux, the total (asymptotic plus transient) scalar flux is continuous across a boundary. This is achieved by introducing another parameter $\alpha(c)$ in the transient flux theory which is determined from the condition that the total flux gives exact transport-theory leakage from a constant source Milne problem. This excellent theory proposed by Pomraning has, however, certain limitations. Although boundary conditions have been modified through introduction of different parameters, a generalized modified boundary condition has not been prescribed. This was not possible because the formalism did not go beyond a diffusion-like approximation. Also, the theory is based on replacement of vacuum by purely absorbing medium (i.e. Mark boundary conditions) - the more versatile Marshak boundary conditions were not used. The theory is only concerned with scalar flux - thus improvements on various integral parameters (angle-integrated) were only tested. Some inconsistency is also observed in evaluation of $\Gamma(c)$ for $c > 1$, and $\alpha(c)$ cannot be calculated for $c > 1$. Calame [27] prescribed alternate sets of parameters for use in Pomraning's diffusion-transport equation to give flux transients at an interface and near source accurately. Doyas and Koponen [28] extended the asymptotic neutron diffusion theory to linear anisotropic case. They suggested and evaluated anisotropic transport-theory corrections to asymptotic diffusion theory. The improvement of general P_N-approximation along with the work on asymptotic diffusion theory was also in progress.

Conkie [29] gave several iterative schemes to improve the conventional P_N-approximation. In his analysis, iteration procedure started with the P_N-approximation value of the angle-integrated flux. The idea was that the total flux is determined more accurately than the higher angular moments, since it is an integral over the approximate angular distribution and presumably the error in the angular distribution is oscilatory because of orthogonal function expansion. It was also possible to satisfy the exact boundary condition of the problem. In his later paper, Pomraning [30] presented an approximation to the transport equation which yields the exact transport theory asymptotic behaviour in all orders for any geometry and is accurate to any arbitrary degree. The approximation, very similar to the usual spherical harmonics method is derived by introducing a new truncation scheme into the infinite set of spherical harmonics equations. The truncation method consists of assuming that the higher spherical harmonics components, equated to zero in the P_N-method, can be related to lower components by assuming the angular distribution to be in an asymptotic distribution. The resulting approximation, called as A_N approximation, is not more complex than the usual spherical harmonics method for computational purposes. The (N+1)-th spherical harmonics equation in slab geometry is given as

$$(N+1)\frac{d\,\phi_{N+1}(x)}{dx} + (2n+1)\,\phi_N(x) + N\frac{d\,\phi_{N-1}(x)}{dx} = 0 \tag{1.4}$$

where,

$$\phi_n(x) = 2\pi\int_{-1}^{1} d\mu\, P_n(\mu)\,\psi(x,\mu) \tag{1.5}$$

If the angular distribution $\psi(x,\mu)$ in equation (1.5) is assumed to be in its asymptotic form as

$$\psi(x,\mu) = \frac{A\,e^{x/\nu}}{1+\mu/\nu} + \frac{B\,e^{-x/\nu}}{1-\mu/\nu} \tag{1.6}$$

where A and B are arbitrary constants. By use of equations (1.5) and (1.6) a relation between $\phi_{N+1}(x)$ and $\phi_{N-1}(x)$ is derived as

$$\phi_{N+1}(x) = \bar{\alpha}_N\,\phi_{N-1}(x) \tag{1.7}$$

where,

$$\bar{\alpha}_N = \frac{\int_{-1}^{1} d\mu\, P_{N+1}(\mu)\,\frac{1}{(1+\mu/\nu)}}{\int_{-1}^{1} d\mu\, P_{N-1}(\mu)\,\frac{1}{(1+\mu/\nu)}}$$

$\phi_{N+1}(x)$ in equation (1.4) is now replaced by relation (1.7). Introducing a parameter γ_N as,

$$\gamma_N = 1 + \left(\frac{N+1}{N}\right) \bar{\alpha}_N$$

this process is equivalent to setting $\phi_{N+1}(x)$ equal to zero and replacing $\phi_{N-1}(x)$ by $\gamma_N \phi_{N-1}(x)$ in equation (1.4). Copic [31] extended Pomraning's work to give an explicit expression for the ratio of (N+1)-th to (N-1)-th angular moments i.e. $\bar{\alpha}_N$. Following Davison [4], he also showed that the attenuation distances of the remaining solutions (i.e. the transient component) in the finite order approximation are all shorter than the diffusion length as given by the asymptotic eigenvalue. The eigenvalues in the A_N-approximation are given by a certain determinental condition just like the case of usual spherical harmonics method. Although the largest eigenvalue gives the exact asymptotic behavior, it has not been shown in Pomraning's theory that the remaining $\frac{1}{2}(N-1)$ pair of eigenvalues for odd order approximation are confined in the interval (-1, 1). The behaviour of A_N-approximation as $N \to \infty$ was not also investigated. An analytic transient flux expression for use with asymptotic diffusion theory is prescribed by Beghian [32] in his treatment of monoenergetic integral transport equation. The exponential transient representation is replaced by exponential integrals to yield significantly improved results over diffusion theory. Summarising, it can be said that the improvement on conventional P_N approximation proceeded along two parallel paths: one was the development of asymptotic diffusion theory by replacing the diffusion parameters like decay constant, diffusion coefficient by their transport theory values. This was mostly achieved by either ad-hoc intuitive basis or variational formulation. The other was on development of improved general P_N-theory with transient components included. Unfortunately, the development in this direction lacks an unified and consistent approach. In many cases, systematic construction of higher order approximation is not possible. Most of the theories are concerned with scalar flux except perhaps Pomraning's A_N theory which deals with angular flux. However, the theory has its limitations as pointed out earlier.

1.2 Outline and Objective of Thesis:

It has been outlined in the previous section that the present work on one-speed neutron transport theory is centered around the spherical harmonics method and Case's singular eigenfunction expansion method. It is true that the P_N-approximation cannot be a competitor to the versatile S_N-method for practical reactor calculations, but the former method has some plus points in some cases. The beauty of P_N-approximation is that it can provide the functional behaviour of angular neutron density while the S_N method deals with discrete numbers only. Due to this factor, the old spherical harmonics method has regained its lost impetus in recent times- as for example, the prediction of functional behaviour of neutron angular density deep within a medium by Kin [33] in his dissertation. The improvement of conventional P_N-approximation is necessiated by faster convergence of solution. From what has been sketched in the previous section, it can be concluded that while the state of art has proceeded remarkably in scalar flux improvement by replacement of diffusion parameters by their transport theory counterparts and by allowing some discontinuity in flux or current or in both at an interface, the general improvement of P_N-approximation through better representation of angular flux by modification of usual boundary conditions has not received proper attention. The present work is an attempt towards a better angular flux representation. The main objective in this work is i) to demonstrate that the use of all the roots of P_N-approximation is not mathematically justified and hence, by implication, it is the transport theoretic ν_0 which should be incorporated in place of asymptotic decay constant of P_N-approximation,

ii) to generalize the conventional Marshak free-surface boundary condition in order to get the fullest advantage of the use of exact ν_o. As it will be seen in the analysis, the first part is achieved by suitable construction of $g_n(\nu)$ functions as they appear in P_N-theory both in the ranges of $\nu \notin (-1, 1)$ and $\nu \varepsilon (-1, 1)$. Modification of boundary conditions is realized by introduction of a parameter $\alpha_N(c)$ in the first equation of the set of Marshak boundary conditions. $\alpha_N(c)$ is evaluated by forcing the asymptotic flux for the source-free Milne problem to be identically same as exact transport theory asymptotic flux. The Milne problem is chosen as a reference problem as it leads to the natural free-surface boundary conditions. The same α_N can be used for any other transport problem involving a free surface. The solution is constructed with the asymptotic part being of the same nature as exact solution and the transient part terminated as in conventional P_N-approximation. Since the transient is in the framework of P_N-approximation, unlike previous attempts, construction of any order of approximation is possible in the present approach. Interface boundary conditions, which are more useful for practical reactor calculations, are also modified in the proposed TP_N theory. In a two-media Milne problem the modification is achieved by demanding an exact asymptotic behaviour in the right hand side when the adjacent medium is replaced by a purely absorbing one. It is expected in general that through exact angular representation of flux, atleast for the asymptotic part, the convergence of solution can be achieved in a reasonably lower order of approximation. However, due to inadequate transient flux representation, the TP_N-approximation does not necessarily improve the P_N result in those cases where transient is overwhelmingly predominant. This calls for a better transient flux representation and it is felt that this may not be possible within the framework of P_N-approximations. Finally, it is to be concluded that the different inferences drawn in the present analysis, like replacement of different P_N-approximation parameters by their transport-theory counterparts, are not just adhoc prescriptions but are justified by rigorous mathematical formulation.

As has been remarked in the last section, all standard one-speed transport theory problems have been analyzed by Case's exact theory in great detail. Thus, from calculational point of view, it is not worthwhile to compete with the existing methods of solving these problems. It is only some general mathematical problems associated with Case's method that need attention. In neutron transport theory, eigenvalue problems occur repeatedly in different contexts where the existence of dominant eigenvalue is of great importance. Proper mathematical study of such a problem was pioneered by Lehner and Wing [34] in their analysis of one-speed time dependent transport equation in a finite slab. The equation is transformed into an eigenvalue equation of the form

$$\phi(x) = \frac{\gamma}{2} \int_{-a}^{a} E_1(\lambda|x - x'|)\, \phi(x')\, dx' \tag{1.8}$$

Equation (1.8) can be viewed as an inverse eigenvalue equation in the sense that the eigenvalue $\gamma/2$ is known and the parameter λ (spectrum of one-speed operator) which has to be determined is in the kernel of the integral equation. The task would have been easier if λ were fixed and $\gamma/2$ were to be determined! By means of classical approach, Lehner and Wing were able to prove the following result – the Boltzmann operator decomposes the λ – plane into i) point spectrum – a finite non-empty set lying on $\lambda > 0$ ii) continuous spectrum – the real line $\mathrm{Re}(\lambda) \leq 0$, iii) residual spectrum – empty, iv) resolvent set $\mathrm{Re}(\lambda) > 0$ deleted by the point spectrum. The existence of a dominant eigenvalue was established by establishing a proper ordering among the discrete eigenvalues of the point spectrum. In his study of time dependent slowing down equation (space independent) Ukai [35] gets an equation similar to equation (1.8) of Lehner and Wing as

$$\rho\, \phi(v) = \int_0^{\infty} G_\lambda (v, v') \, \phi(v') \, dv' \tag{1.9}$$

where v is the velocity variable. Ukai proceeds by fixing λ arbitrarily and solves equation (1.9) to obtain a set of eigenvalues, ρ_n. Each eigenvalue ρ contains λ as a parameter so that ρ is denoted as $\rho(\lambda)$. From equation (1.9) it is evident that the parameter λ is given by the solution of the equation $\rho(\lambda) = 1$. Functional analytic studies on general Boltzmann operator A were also made by several authors [36-38]. In this case, it was found that i) the whole half-plane $\mathrm{Re}(\lambda) \leq -\lambda^* = \min [v\, \Sigma(r, v)]$ belongs to continuous spectrum of the Boltzmann operator, ii) there exists a number c_o such that the half-plane $\mathrm{Re}(\lambda) > c_o$ lies in the resolvent set of A and iii) the points of the strip $-\lambda^* < \mathrm{Re}(\lambda) \leq c_o$ also belongs to the resolvent set $\rho(A)$ with the exception of a set of isolated eigenvalues which constitute the point spectrum. In his analysis, Vidav [36] applied a theorem from functional analysis to establish the existence of a fundamental mode of decay if the set of λ_k is not empty. The existence of corresponding non-negative unique eigenfunction was proved by application of a theorem by Krein and Rutmann [39]. Similar analysis in a more general way can be found in a paper by Larsen and Zweifel [37]. In Chapter III of the present work, the two coupled Fredholm equations in terms of the discrete and continuous coefficients arising in a finite slab criticality problem are coupled together to form a single integral equation. The problem is then posed as an inverse eigenvalue problem in which the eigenvalue is given and the operator $\mathbb{K}$ has to be determined. By application of functional analytic theorems in the range of analyticity of the operator-valued function $\mathbb{K}(b)$ (b is the inverse eigenvalue parameter), the existence of critical thickness is proved. Analyticity criterion on $\mathbb{K}(b)$ shows that the critical thickness b_c must be less than the end-point result. This fact is not reflected by P_N-calculation. Estimates of spectral radius in its simplest form are used for numerical calculation of critical thickness. It was necessary to depart from the original problem slightly because of restriction of positivity criterion on the kernel of the integral equations. This is because the relevant theorems are valid for positive operators only. As calculations will reveal, the results obtained are fairly accurate in spite of dealing with the approximate problem. The choice of the criticality problem was made as this problem has not been seen in this light. Also, the present analysis is based on a more broad-based mathematical theory. The numerical results in this work were obtained only to substantiate the hypothesis adopted in the formulation. No sophistication in calculational technique has been attempted to improve the numerical results, because our main aim was not to calculate critical thickness (which has been done to great accuracies earlier) but to formulate and solve a class of inverse eigenvalue problems. Thus the present calculational method does not claim to be a competitor to the fast converging Neumann series solution for critical thickness. However, in those cases where the numerical values of inverse eigenvalue parameter are not otherwise easily available, the present method of calculation may be adopted.

CHAPTER II

A TRANSPORT THEORETIC P_N-APPROXIMATION

Introduction

In Chapter I, an outline of the present state of P_N-approximation is given. As has been noticed, most of the works on improvement of conventional P_N-approximation deal with scalar flux and they are diffusion-like approximations. In this chapter, we give an improved approximate scheme that can yield better angular flux representation and can be easily adopted for higher order approximations beyond P_1 approximation. To realise this, the discretization procedure of eigenvalue spectrum in conventional P_N-approximation is modified. This is necessiated by the mathematical analysis that follows in the development of the first part of the theory. Simultaneously in the second part of the proposed theory, the usual free-surface boundary conditions are modified to achieve better angular flux representation. The improved scheme in general can be applied for any problem involving a free surface. The usual interface boundary condition of continuity of moments of angular neutron density is also suitably changed in the proposed analysis. Formal solution of the transport equation is then constructed with the asymptotic part being of the same nature as exact solution and the transient terminated as in conventional P_N-approximation. The complete formalism is called transport theoretic P_N-approximation and this approximation will be referred as TP_N approximation. This chapter ends with numerical calculation of different standard one-speed neutron transport problems by TP_N method.

2.1 Analysis

The one-speed transport equation in slab-geometry with isotropic scattering is

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \Sigma \psi(x, \mu) = \frac{c\Sigma}{2} \int_{-1}^{1} \psi(x, \mu') \, d\mu' \qquad (2.1)$$

In Case's exact analysis, the solution of equation (2.1) can be written when $c \neq 1$, as

$$\psi(x, \mu) = a_{o+} e^{-\Sigma x/\nu_o} \phi_{o+}(\mu) + a_{o-} e^{\Sigma x/\nu_o} \phi_{o-}(\mu) + \int_{-1}^{1} A(\nu) e^{-\Sigma x/\nu} \phi_\nu(\mu) \, d\nu \qquad (2.2)$$

where,

$$\phi_{o\pm}(\mu) = \frac{c\nu_o}{2} \frac{1}{\nu_o \mp \mu} \qquad (2.3)$$

ν_o in equation (2.3) is a solution of

$$\frac{c\nu}{2} \ln \frac{\nu+1}{\nu-1} = 1 \qquad (2.4)$$

and, if $\nu \in (-1, 1)$

$$\phi_{\nu}(\mu) = \frac{c\nu}{2} P \frac{1}{\nu - \mu} + \lambda(\nu)\, \delta(\nu - \mu) \qquad (2.5)$$

In equation (2.5), P denotes the Cauchy principal value. The main difference between equations (2.3) and (2.5), besides the principal value, is the appearance of the extra-factor involving the arbitrary function $\lambda(\nu)$. This fact will prove to be important in the analysis to follow on the spherical harmonics approximation.

In the spherical harmonics method $\psi(x, \mu)$ is written,as

$$\psi(x, \mu) = \sum_{n=0}^{\infty} \left(\frac{2n+1}{2}\right) \psi_n(x)\, P_n(\mu) \qquad (2.6)$$

Assuming $\psi_n(x) = g_n(\nu)\, e^{-\Sigma x/\nu}$, the above becomes

$$\psi(x, \mu) = e^{-\Sigma x/\nu} \sum_{n=0}^{\infty} \left(\frac{2n+1}{2}\right) g_n(\nu)\, P_n(\mu) \qquad (2.7)$$

In exact treatment the infinite sum in equation (2.7) is denoted by $\phi_\nu(\mu)$ i.e.,

$$\phi_{\nu}(\mu) = \sum_{n=0}^{\infty} \left(\frac{2n+1}{2}\right) g_n(\nu)\, P_n(\mu) \qquad (2.8)$$

The coefficients $g_n(\nu)$ in the expansion of $\phi_\nu(\mu)$ can be obtained simply as

$$g_n(\nu) = \int_{-1}^{1} \phi_\nu(\mu)\, P_n(\mu)\, d\mu \qquad (2.9)$$

By use of equations (2.3) and (2.5), we get from eqn.(2.9)

$$g_n(\nu) = c\nu Q_n(\nu), \quad \nu \notin (-1, 1) \tag{2.10}$$

$$= c\nu P Q_n(\nu) + \lambda(\nu) P_n(\nu), \quad \nu \in (-1, 1) \tag{2.11}$$

The functions $Q_n(\nu)$ are the Legendre polynomials of second kind and are defined as

$$Q_n(\nu) = \frac{1}{2} \int_{-1}^{1} \frac{P_n(\mu)}{(\nu - \mu)} d\mu, \quad \nu \notin (-1, 1) \tag{2.12}$$

and,

$$P\, Q_n(\nu) = \frac{1}{2} P \int_{-1}^{1} \frac{P_n(\mu)}{(\nu - \mu)} d\mu, \quad \nu \in (-1, 1) \tag{2.13}$$

When $\nu \in (-1, 1)$, principal value integration is used because of singularity at $\mu = \nu$. For this range of ν, Q_n functions will be denoted as $PQ_n(\nu)$. A brief discussion on these functions is pertinent to the present analysis. The functions $Q_n(\nu)$ like $P_n(\nu)$ are oscillatory in the interval $(-1, 1)$ and possess zeroes there, but like $P_n(\nu)$, they are monotonic functions outside this interval. For example, when $n = 0$

$$Q_o(\nu) = \frac{1}{2} \ln \frac{\nu+1}{\nu-1}, \quad \nu \notin (-1, 1)$$

and,

$$Q_o(\nu) = \frac{1}{2} \ln \frac{1+\nu}{1-\nu}, \quad \nu \in (-1, 1)$$

It is seen that $Q_o(\nu)$ possesses zero at $\nu = 0$ for $\nu \in (-1, 1)$, but does not have a zero for $\nu \notin (-1, 1)$. The $Q_n(\nu)$ functions satisfy the same recurrence relation as the $P_n(\nu)$,

$$(n+1)\, Q_{n+1}(\nu) = (2n+1)\, \nu Q_n(\nu) - n\, Q_{n-1}(\nu), \quad n \geq 1 \tag{2.14}$$

With the knowledge of $Q_o(\nu)$ and $Q_1(\nu)$, $Q_n(\nu)$ for $n > 1$ can be evaluated from equation (2.14). $Q_1(\nu)$ can be obtained from equation (2.12) or (2.13) as

$$\begin{aligned} Q_1(\nu) &= \nu Q_o(\nu) - 1 && \nu \notin (-1, 1) \\ &= \nu P Q_o(\nu) - 1 && \nu \in (-1, 1) \end{aligned}$$

$Q_n(\nu)$ can also be expressed in terms of $P_n(\nu)$ by the following continued fraction expression

$$\frac{Q_n(\nu)}{P_n(\nu)} = Q_o(\nu) - \frac{1}{\nu -}\; \frac{1}{3\nu -}\; \frac{4}{5\nu -} \cdots - \frac{(n-1)^2}{(2n-1)\nu}$$

Another interesting property of $Q_n(\nu)$ is that $Q_n(\nu) \to 0$ as $n \to \infty$ for all ν.

The normalization condition $\int_{-1}^{1} \phi_\nu(\mu)\, d\mu = 1$ for all ν implies $g_o(\nu) = 1$. For $\nu \notin (-1, 1)$, this gives Case's transcendental equation (2.4) the solution of which are the pair of asymptotic decay constants $\pm \nu_o$, while for $\nu \in (-1, 1)$, this determines the form of ν

dependence of $\lambda(\nu)$:

$$\lambda(\nu) = 1 - c\nu P Q_o(\nu)$$

With this value of $\lambda(\nu)$, the expression for $g_n(\nu)$ in the range $\nu \varepsilon (-1, 1)$ is that given in Davison [4]. However, the present analysis shows that this expression for $g_n(\nu)$ is valid only when $\nu \varepsilon (-1, 1)$. The conventional P_N-approximation involves approximation of equation (2.8) by a finite sum i.e.,

$$g_{N+1}(\nu) = 0 \tag{2.15}$$

The equation (2.15) forms the basis of P_N-approximation. The general solution in such an approximation is constructed as

$$\psi(x, \mu) = \sum_{j=\text{roots}} a_j^{(N)} e^{-\Sigma x/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \tag{2.16}$$

where the entire range of ν is suitably discretised.

It is obvious that $g_n(\nu)$ of eqn. (2.8) cannot be zero for any finite $n = N$ because the Legendre polynomials are an infinite set of orthogonal polynomials. (Eqns. (2.10) and (2.11) ofcourse satisfy the condition $g_n(\nu) = o$ as $n \to \infty$). Any attempt to set $g_{N+1}(\nu) = 0$ can, therefore, result in possible inconsistencies. Thus, Davison [4] obtains the largest root (asymptotic) less than 1 for small values of c. Looking from equations (2.10) and (2.11), the above follows in a straightforward manner. When ν is outside the interval (-1, 1), $g_n(\nu)$ is given by equation (2.10). The properties of $Q_n(\nu)$ show that it is impossible to satisfy condition (2.15) when $\nu \notin (-1, 1)$. Thus the roots outside (-1, 1) (i.e. the asymptotic roots) can never be found from the condition (2.15) and must always be evaluated from the normalization condition

$$g_o = c\nu_o Q_o(\nu) = 1 \tag{2.17}$$

In the range of $\nu \in (-1, 1)$, it can be shown with the properties of $Q_n(\nu)$ functions that the expression for $g_{N+1}(\nu)$ of equation (2.11) reduces to a polynomial of (N+1)-th order. This polynomial must have (N+1)/2 pair of zeroes and thus the condition (2.15) can be satisfied in the range of $\nu \in (-1, 1)$. However, since equation (2.15) in this case has the required (N+1) roots, two of them must be redundant as they have been already obtained from equation (2.17). It is known that equation (2.15) can admit largest pair of roots both greater or less than 1 [4]. When greater than 1, this pair is straightaway rejected as equation (2.11) is valid only for $\nu \in (-1, 1)$. However, the inclusion of the largest root when it is less than 1 is not also possible as this would lead to consideration of two extra roots. We, therefore, conclude that, irrespective of the value of largest roots, only the smallest (N-1) roots of equation (2.15) (where eqn. (2.11) is used for $g_n(\nu)$) should be used to describe the transient flux while the asymptotic flux has to be constructed from the roots obtained from eqn.(2.17). In his analysis, Hendry [40] neglects the roots greater than 1 but retains them as two extra 'basis functions' when they are in the transient range. This is, however, not true as the two additional roots do not generate extra basis functions; the orthonormal basis functions in the present case are the Legendre polynomials and not the spatial modes exp $(-x/\nu)$. The present analysis also establishes an exact relationship between (N+1)-th moment to (N-1)-th moment of angular flux, a quantity used by Pomraning [30] in his A_N approximation theory. The parameter $\bar{\alpha}_N$, as defined by Pomraning is

$$\bar{\alpha}_N = \frac{Q_{N+1}(\nu)}{Q_{N-1}(\nu)}$$

From eqn. (2.8) it follows,

$$\bar{\alpha}_N = \frac{g_{N+1}(\nu)}{g_{N-1}(\nu)}$$

$$= \frac{\phi_{N+1}(x)}{\phi_{N-1}(x)}$$

by definition. Thus, the replacement of $\phi_{N+1}(x)$ by $\bar{\alpha}_N \ \phi_{N-1}(x)$ in N-th eqn. of P_N-approximation will obviously lead to correct asymptotic behaviour of neutron flux.

In Appendix, $g_n(\nu)$ functions are constructed for anisotropic scattering.

2.2 Free Surface Boundary Condition:

The replacement of P_N value of the asymptotic decay constant by its exact value modifies the P_N-solution to $(\Sigma = 1)$,

$$\begin{aligned}\psi(x, \mu) = {} & a_{o+}^{(N)} e^{-x/\nu_o} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_o) P_n(\mu) \\ & + a_{o-}^{(N)} e^{x/\nu_o} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(-\nu_o) P_n(\mu) \\ & + \sum_{j=\text{roots}} A_j^{(N)} e^{-x/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu)\end{aligned}$$

where ν_j are (N-1) roots corresponding to the transient flux and are obtained from solutions of eqns.(2.11) and (2.15). However, considering the poor convergence of the Legendre Polynomial series in n,[41] we wish to go further and thus retain the infinite sums for the asymptotic roots and terminate the series for the transient part only. Hence the general solution changes as

$$\begin{aligned}\psi(x, \mu) = {} & a_{o+}^{(N)} e^{-x/\nu_o} \phi_{o+}(\mu) + a_{o-}^{(N)} e^{x/\nu_o} \phi_{o-}(\mu) \\ & + \sum_{j=\text{roots}} A_j^{(N)} e^{-x/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu)\end{aligned} \tag{2.18}$$

The coefficients in eqn. (2.18) are to be evaluated from the boundary conditions. Equation (2.18) shows that asymptotic part of the flux in this case is of exact nature, and can indeed be made equal to its exact value by suitable modification of boundary conditions. But in order to do so, the boundary condition has to be changed for each problem to ensure exact asymptotic flux in each case. This idea is not practically applicable. To generalize concept, we wish to get the exact extrapolated end point and modify the free surface Marshak boundary condition. Since the source-free Milne problem defines the extrapolation end-point, where the asymptotic scalar flux vanishes, the modification of the Marshak boundary conditions at the free surface will make the asymptotic coefficient $a_{0+}^{(N)}$ equal to its exact value a_{0+} for the Milne problem. The modified form of Marshak boundary condition is then applied for any other problem involving a free-surface. While for source-free Milne problem the asymptotic flux will be exact by definition, the same will not be true for other problems but will definitely be an improvement. This conclusion will be reflected by numerical calculations of different standard one-speed problems given at the end of the chapter.

2.3 Source-Free Milne Problem and Modified Boundary Conditions

The exact solution of the source-free Milne problem is

$$\psi(x,\ \mu) = a_{0+}\ e^{-x/\nu_0}\ \phi_{0+}(\mu) + e^{x/\nu_0}\ \phi_{0-}(\mu)$$

$$+ \int_0^1 A(\nu)\ e^{-x/\nu}\ \phi_\nu(\mu)\ d\nu \qquad (2.19)$$

where,

$$a_{0+} = \frac{X(-\nu_0)}{X(\nu_0)} = -e^{-2z_0/\nu_0} \qquad (2.20)$$

where $X(\nu_0)$ is the well-known X - function of Case's theory and is defined by the eqn. [42]

$$X(z) = \frac{c}{2}\ \frac{1}{1-c} \int_{-1}^{0} \frac{\mu'}{(\nu_0^2 - \mu'^2)}\ \frac{1}{X(\mu')}\ \frac{d\mu'}{\mu'+z}$$

$z_0(c)$ is the exact extrapolated end point and is tabulated by Case, de Hoffmann and Placzek [23].

The associated free-surface boundary condition is

$$-\phi_{0-}(\mu) = a_{0+}\ \phi_{0+}(\mu) + \int_0^1 A(\nu)\ \phi_\nu(\mu)\ d\nu \quad , \ \mu \geq 0$$

$$(2.21)$$

In the present case, the exact solution as given by eqn.(2.19) changes to

$$\psi(x, \mu) = a_{0+} e^{-x/\nu_0} \phi_{0+}(\mu) + e^{x/\nu_0} \phi_{0-}(\mu) + \sum_{j=\text{roots}}' A_j^{(N)} e^{-x/\nu_j} \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \tag{2.22}$$

The associated free-surface condition is

$$-\phi_{0-}(\mu) = a_{0+} \phi_{0+}(\mu) + \sum_{j=\text{roots}}' A_j^{(N)} \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \tag{2.23}$$

where, prime in the summation indicates that only positive roots are considered.

The condition (2.21) is obtained from the exact free-surface conditions $\psi(x, \mu)|_{x=0} = 0$, $\mu \geq 0$. Since $\phi_{0+}(\mu)$ and $\phi_\nu(\mu)$ form a complete set in case of half-space problem, a_{0+} and $A(\nu)$ of eqn.(2.21) can be exactly evaluated from half range orthogonality relations. Because of truncation in the transient part, eqn. (2.23) cannot, however, beexactly satisfied. In the conventional Marshak boundary condition, P_n moments $(n = 1, 3, \ldots N)$ of $\psi(0, \mu)$ are only made equal to zero and these equations are used to evaluate the coefficients. Since $\phi_{0\pm}(\mu)$ of eqn.(2.23) are infinite series in Legendre polynomials (eqn.(2.8)), the Legendre polynomials are still the basis functions in the present case. Therefore, in the modified version of the free surface boundary condition the P_n moments of $\psi(0, \mu)$ are to be used. However, in the present formalism the number of unknowns are reduced to (N-1) as the asymptotic coefficient is forced to its exact value. Thus, it is necessary to introduce a parameter $\alpha_N(c)$ in the first of the set of Marshak boundary conditions so that a_{0+} is indeed given by eqn.(2.20). $\alpha_N(c)$ will be evaluated from the condition of exactness of asymptotic coefficient. The detailed analysis is given below. The conventional Marshak boundary condition is

$$\int_0^1 P_n(\mu)\,\psi(o, \mu)\,d\mu = 0 \qquad n = 1,3,5\ldots N \tag{2.24}$$

The modified free-surface condition becomes,

$$\int_0^1 (\mu + \alpha_N)\,\psi(0, \mu)\,d\mu = 0 \tag{2.25a}$$

$$\int_0^1 P_n(\mu)\,\psi(0, \mu)\,d\mu = 0 \qquad n = 3,5\ldots N \tag{2.25b}$$

i.e. instead of taking $\{P_n(\mu)_{\;n=1,3,5\ldots N}\}$ moments, we take here $\{(\mu+\alpha),\ P_n(\mu)_{\;n=3,5,\ldots N}\}$ moments of $\psi(0, \mu)$. The use of (2.25) in eqn.(2.23) yields,

$$c\nu_o \int_o^1 \frac{(\mu + \alpha_N)}{(\nu_o + \mu)} d\mu + a_{o+} \, c\nu_o \int_o^1 \frac{(\mu + \alpha_N)}{(\nu_o - \mu)} d\mu$$

$$+ \sum_j{}' A_j^{(N)} \sum_{n=o}^{N} (2n+1) \, g_n(\nu_j) \int_o^1 (\mu+\alpha_N) \, P_n(\mu) \, d\mu = 0 \qquad (2.26a)$$

and

$$c\nu_o \int_o^1 \frac{P_m(\mu)}{(\nu_o + \mu)} d\mu + a_{o+} \, c\nu_o \int_o^1 \frac{P_m(\mu)}{(\nu_o - \mu)} d\mu$$

$$+ \sum_j{}' A_j^{(N)} \sum_{n=o}^{N} (2n+1) \, g_n(\nu_j) \int_o^1 P_m(\mu) \, P_n(\mu) \, d\mu = 0$$

$$m = 3,5,\ldots N \qquad (2.26b)$$

Equations (2.26a) and (2.26b) are $(\frac{N+1}{2})$ equations in the unknown α_N and $(\frac{N-1}{2})$ coefficients $A_j^{(N)}$. It is to be noted that a_{o+} in this case is known and is given by eqn. (2.20). α_N thus obtained is used for all problems involving half-space. The formalism is now complete and the present scheme will, henceforth, be called as TP_N approximation. In the next section, the evaluation of α_N for TP_1 and TP_3 are presented.

2.4 $\alpha_N(c)$ for TP_1 and TP_3 Approximations

In the TP_1 approximation, we have

$$\int_0^1 \frac{(\mu + \alpha_1)}{(\nu_0 + \mu)} \, d\mu + a_{0+} \int_0^1 \frac{(\mu + \alpha_1)}{(\nu_0 - \mu)} \, d\mu = 0$$

i.e.
$$a_{0+} = \frac{(\nu_0 - \alpha_1) \ln \frac{\nu_0 + 1}{\nu_0} - 1}{(\nu_0 + \alpha_1) \ln \frac{\nu_0}{\nu_0 - 1} - 1}$$

By use of eqn. (2.20), we get,

$$-e^{-2z_0/\nu_0} = \frac{(\nu_0 - \alpha_1) \ln \frac{\nu_0 + 1}{\nu_0} - 1}{(\nu_0 + \alpha_1) \ln \frac{\nu_0}{\nu_0 - 1} - 1}$$

or,
$$-\frac{e^{-z_0/\nu_0}}{e^{-z_0/\nu_0}} = \frac{(\nu_0 - \alpha_1) \ln \frac{\nu_0 + 1}{\nu_0} - 1}{(\nu_0 + \alpha_1) \ln \frac{\nu_0}{\nu_0 - 1} - 1}$$

$$\frac{e^{z_0/\nu_0} - e^{-z_0/\nu_0}}{e^{z_0/\nu_0} + e^{-z_0/\nu_0}} = \frac{\nu_0 \ln \frac{\nu_0 + 1}{\nu_0 - 1} + \alpha_1 \ln \frac{\nu_0^2}{\nu_0^2 - 1} - 2}{\alpha_1 \ln \frac{\nu_0 + 1}{\nu_0 - 1} + \nu_0 \ln \frac{\nu_0^2}{\nu_0^2 - 1}}$$

For $c < 1$, the left hand side is tanh (z_0/ν_0) and for $c > 1$, by using $\nu_0 = ik_0$, it becomes tan (z_0/k_0). Also, by definition the linear extrapolation length $\lambda(c)$ is given as,

$$\lambda(c) = \nu_o \tanh (z_o/\nu_o), \qquad c < 1$$

$$= k_o \tan (z_o/k_o), \qquad c > 1$$

Thus, when c < 1, we get

$$\lambda(c) = \frac{2\nu_o^2(1-c) + \alpha_1 c \nu_o^2 \ln \frac{\nu_o^2}{\nu_o^2-1}}{2\alpha_1 + c\nu_o^2 \ln \frac{\nu_o^2}{\nu_o^2-1}}, \qquad (2.27)$$

and when c > 1,

$$\lambda(c) = - \frac{2k_o^2 (1-c) - \alpha_1 c k_o^2 \ln \frac{k_o^2+1}{k_o^2}}{2\alpha_1 + c k_o^2 \ln \frac{k_o^2+1}{k_o^2}} \qquad (2.28)$$

$\alpha_1(c)$ is obtained from (2.27) and (2.28) as

$$\alpha_1(c) = \nu_o^2 \frac{2(1-c) - c\lambda(c) \ln \frac{\nu_o^2}{\nu_o^2-1}}{2\lambda(c) - c\nu_o^2 \ln \frac{\nu_o^2}{\nu_o^2-1}}, \quad c < 1 \qquad (2.29)$$

and,

$$\alpha_1(c) = k_o^2 \frac{2(c-1) - c\lambda(c) \ln \frac{k_o^2+1}{k_o^2}}{2\lambda(c) - ck_o^2 \ln \frac{k_o^2+1}{k_o^2}}, \quad c > 1 \qquad (2.30)$$

In TP_3 approximation, the boundary conditions in our formalism are,

$$c\nu_o \int_o^1 \frac{(\mu+\alpha_3)}{(\nu_o+\mu)}\,d\mu + a_{o+}\, c\nu_o \int_o^1 \frac{(\mu+\alpha_3)}{(\nu_o-\mu)}\,d\mu$$

$$+ A_1^{(3)} \sum_{n=o}^{3} (2n+1)\, g_n(\nu_1) \int_o^1 (\mu+\alpha_3)\, P_n(\mu)\, d\mu = 0 \tag{2.31}$$

and,

$$c\nu_o \int_o^1 \frac{P_3(\mu)}{(\nu_o+\mu)}\,d\mu + a_{o+}\, c\nu_o \int_o^1 \frac{P_3(\mu)}{(\nu_o-\mu)}\,d\mu$$

$$+ A_1^{(3)} \sum_{n=o}^{3} (2n+1)\, g_n(\nu_1) \int_o^1 P_n(\mu)\, P_3(\mu)\, d\mu = 0 \tag{2.32}$$

To evaluate the integrals of the type $\int_o^1 \frac{P_n(\mu)}{(\nu_o-\mu)}\,d\mu$, following results are used [43]

$$I_+^{(n)} = \int_o^1 \frac{\mu^n}{(\nu_o+\mu)}\,d\mu = \frac{1}{n}\left(1-n\nu_o\, I_+^{(n-1)}\right)$$

$$I_-^{(n)} = \int_o^1 \frac{\mu^n}{(\nu_o-\mu)}\,d\mu = -\frac{1}{n}\left(1-n\nu_o\, I_-^{(n-1)}\right)$$

with, $I_+^{(0)} = \ln \frac{\nu_o+1}{\nu_o}$ and $I_-^{(0)} = \ln \frac{\nu_o}{\nu_o-1}$.

Thus,

$$\int_0^1 \frac{P_3(\mu)}{(\nu_0 \pm \mu)}\, d\mu = \frac{5}{2}\, I_{\pm}^{(3)} - \frac{3}{2}\, I_{\pm}^{(1)}$$

Carrying out the integrations in eqns. (2.31) and (2.32), these equations simplify to

$$\begin{aligned} & c\nu_0 \left(I_+^{(1)} + \alpha_3\, I_+^{(0)}\right) + a_{0+}\, c\nu_0 \left(I_-^{(1)} + \alpha_3\, I_-^{(0)}\right) \\ & + A_1^{(3)} \left\{ \left(\frac{1}{2} + g_1(\nu_1) + \frac{5}{8}\, g_2(\nu_1)\right) \right. \\ & \left. + \alpha_3 \left(1 + \frac{3}{2}\, g_1(\nu_1) - \frac{7}{8}\, g_3(\nu_1)\right) \right\} = 0 \qquad (2.33) \end{aligned}$$

$$\begin{aligned} & c\nu_0 \left(\frac{5}{2}\, I_+^{(3)} - \frac{3}{2}\, I_+^{(1)}\right) + a_{0+}\, c\nu_0 \left(\frac{5}{2}\, I_-^{(3)} - \frac{3}{2}\, I_-^{(1)}\right) \\ & + A_1^{(3)} \left\{ -\frac{1}{8} + \frac{5}{8}\, g_2(\nu_1) + g_3(\nu_1) \right\} = 0 \qquad (2.34) \end{aligned}$$

Eliminating $A_1^{(3)}$ from eqns. (2.33) and (2.34), the expression for $\alpha_3(c)$ is obtained as, with $a_{0+} = -e^{-2z_0/\nu_0}$,

$$\alpha_3(c) = \frac{\beta_{12}(\nu_1)\, f_1(c, \nu_0) + \beta_{23}(\nu_1)\, f_2(c, \nu_0)}{\beta_{23}(\nu_1)\, f_3(c, \nu_0) + \beta_{31}(\nu_1)\, f_4(c, \nu_0)}, \quad c < 1 \qquad (2.35)$$

and

$$\alpha_3(c) = \frac{\beta_{12}(\nu_1)\, \bar{f}_1(c, k_0) + \beta_{23}(\nu_1)\, \bar{f}_2(c, k_0)}{\beta_{23}(\nu_1)\, \bar{f}_3(c, k_0) + \beta_{31}(\nu_1)\, \bar{f}_4(c, k_0)}, \quad c > 1 \qquad (2.36)$$

where,

$$
\begin{aligned}
\beta_{12}(\nu_1) &= \frac{1}{4} + \frac{1}{2} g_1(\nu_1) + \frac{5}{16} g_2(\nu_1) \\
\beta_{23}(\nu_1) &= -\frac{1}{16} + \frac{5}{16} g_2(\nu_1) + \frac{1}{2} g_3(\nu_1) \qquad (2.37) \\
\beta_{31}(\nu_1) &= \frac{1}{2} + \frac{3}{4} g_1(\nu_1) - \frac{7}{16} g_3(\nu_1)
\end{aligned}
$$

and

$$
\begin{aligned}
f_1(c, \nu_o) &= \frac{\nu_o}{2} \lambda(c) \left[3 \ln \frac{\nu_o^2}{\nu_o^2 -1} - 5\left(\nu_o^2 \ln \frac{\nu_o^2}{\nu_o^2 -1} -1\right)\right] \\
&\quad -\nu_o \left\{3\left(\frac{1}{c} - 1\right) - 5 \left[\nu_o^2 \left(\frac{1}{c} -1\right) - \frac{1}{3}\right]\right\} \\
f_2(c, \nu_o) &= \nu_o \lambda(c) \ln \frac{\nu_o^2}{\nu_o^2 -1} - 2\nu_o \left(\frac{1}{c} - 1\right) \\
f_3(c, \nu_o) &= \nu_o \ln \frac{\nu_o^2}{\nu_o^2 -1} - \lambda(c) \ln \frac{\nu_o +1}{\nu_o -1} \\
f_4(c, \nu_o) &= \nu_o \left\{3\left(\frac{1}{c} -1\right) -5 \left[\nu_o^2 \left(\frac{1}{c} -1\right) - \frac{1}{3}\right]\right\} \\
&\quad - \frac{\nu_o}{2} \lambda(c) \left[3 \ln \frac{\nu_o^2}{\nu_o^2 -1}\right. \\
&\quad \left. - 5 \left(\nu_o^2 \ln \frac{\nu_o^2}{\nu_o^2 -1} -1\right)\right] \\
\bar{f}_1(c, k_o) &= - \frac{k_o^2}{2} \lambda(c) \left[- 3 \ln \frac{k_o^2 +1}{k_o^2}\right. \\
&\quad \left. - 5 \left(k_o^2 \ln \frac{k_o^2 +1}{k_o^2} -1\right)\right]
\end{aligned}
$$

$$+ k_o^2 \{-3(1 - \tfrac{1}{c}) - 5[k_o^2 (1 - \tfrac{1}{c}) - \tfrac{1}{3}]\}$$

$$\bar{f}_2(c, k_o) = k_o^2 \lambda(c) \ln \frac{k_o^2 + 1}{k_o^2} - 2k_o^2 (1 - \tfrac{1}{c})$$

$$\bar{f}_3(c, k_o) = k_o^2 \ln \frac{k_o^2 + 1}{k_o^2} - \frac{2}{c} \lambda(c)$$

$$\bar{f}_4(c, k_o) = -k_o^2 \{-3(1 - \tfrac{1}{c}) - 5 [k_o^2(1 - \tfrac{1}{c}) - \tfrac{1}{3}]\}$$

$$- \frac{k_o^2}{2} \lambda(c) [3 \ln \frac{k_o^2+1}{k_o^2} + 5(k_o^2 \ln \frac{k_o^2+1}{k_o^2} - 1)]$$

The procedure for evaluation of $\alpha_N(c)$ in the limiting cases $c = 1$ and $c = 0$ are demonstrated below.

i) $\alpha_1(c)$ and $\alpha_3(c)$ for the case $c = 1$

For $c = 1$, the two asymptotic roots coalese at $\pm \nu_o = \infty$ and the two linearly independent eigenmodes are

$$\psi_1(x, \mu) = \frac{1}{2}$$

$$\psi_2(x, \mu) = \frac{1}{2} (x - \mu)$$

For source-free Milne problem, the general solution for $c = 1$ can be written as,

$$\psi(x, \mu) = \frac{z_o}{2} + \frac{1}{2} (x - \mu) + \sum_j{}' A_j^{(N)} e^{-x/\nu_j}$$

$$\times \sum_{n=o}^{N} (\frac{2n+1}{2}) g_n(\nu_j) P_n(\mu) \qquad (2.38)$$

It is to be noted that z_o, the exact extrapolation length, used in eqn. (2.38) ensures exact asymptotic flux for the source-free Milne problem. The free-surface boundary conditions are obtained from the conditions (2.25). Thus, in TP_1 approximation, the boundary condition is

$$\int_o^1 (\mu + \alpha_1)\ (\frac{z_o - \mu}{2})\ d\mu \quad = \quad 0$$

or, $$\alpha_1(1) \quad = \quad - \frac{3z_o - 2}{3(2z_o - 1)} = - \frac{3\lambda(1) - 2}{3(2\lambda(1) - 1)} \qquad (2.39)$$

For $c = 1$, $z_Q(1) = \lambda(1) = 0.7104$ and $\alpha(1)$ is then evaluated from eqn. (2.39).

For TP_3-approximation the boundary conditions are

$$\int_o^1 (\mu + \alpha_3)\ \{\frac{z_o - \mu}{2} + A_1^{(3)} \sum_{n=o}^{3} (\frac{2n+1}{2})\ g_n(\nu_1)\ P_n(\mu)\}\ d\mu = 0 \qquad (2.40a)$$

and

$$\int_o^1 P_3(\mu)\ \{\frac{z_o - \mu}{2} + A_1^{(3)} \sum_{n=o}^{3} (\frac{2n+1}{2})\ g_n(\nu_1) P_n(\mu)\}\ d\mu = 0 \qquad (2.40b)$$

Eliminating $A_1^{(3)}$ from eqn. (2.40), $\alpha_3(1)$ is obtained as,

$$\alpha_3(1) \quad = \quad - \frac{3\beta_{12}(\nu_1)\ \lambda(1) + 4\beta_{23}(\nu_1)\ [3\lambda(1) - 2]}{3\beta_{31}(\nu_1)\ \lambda(1) + 12\ \beta_{23}(\nu_1)[2\lambda(1) - 1]} \qquad (2.41)$$

It is to be noted that in this case, $g_1(\nu) = 0$ and $\lambda(1) = 0.7104$.

ii) $\alpha_1(c)$ and $\alpha_3(c)$ for $c = 0$

The limiting values of $\alpha_1(c)$ and $\alpha_3(c)$ as $c \to 0$ are evaluated by a limiting procedure.

As $c \to 0$,

$$\frac{1}{\nu_o} = 1-2e^{-2/c}$$

By use of this, we get,

$$\ln \frac{\nu_o^2}{\nu_o^2 - 1} = -\ln\left(1 - \frac{1}{\nu_o^2}\right)$$

$$= \frac{2}{c} - \ln 4$$

So, from eqn. (2.29), with $\lambda(0) = 1$, $\alpha_1(0)$ is obtained as,

$$\alpha_1(0) = \frac{-2c + c \ln 4}{2 - c\left(\frac{2}{c} - \ln 4\right)} = -\frac{2 - \ln 4}{\ln 4} \qquad (2.42)$$

Similarly, in TP_3 approximation, $\alpha_3(0)$ is obtained by a limiting procedure from eqn. (2.35).

$$\alpha_3(0) = -\frac{\beta_{12}(\nu_1)\left(\ln 4 - \frac{7}{6}\right) + \beta_{23}(\nu_1)(2 - \ln 4)}{\beta_{23}(\nu_1)\ln 4 + \beta_{31}(\nu_1)\left(\ln 4 - \frac{7}{6}\right)} \qquad (2.43$$

The numerical values of $\alpha_N(c)$ for various values of c in (0,2) as obtained from eqn. (2.27)-(2.30) and (2.39), (2.41)-(2.43) are given in Table 2.1. Due to extreme insensitivity of ν_o on c when c is very small, it is recommended that $\alpha_N(c)$ be obtained by linear interpolation between $0.0 \leq c \leq 0.2$ in both TP_1 and TP_3 approximations. Though it is possible to evaluate α_N for higher order approximations ($N > 3$) in a similar manner, the algebraic complexity of the expressions increases prohibitively. To get around this difficulty, we postulate that $\alpha_N(c)$ varies linearly with $1/N$ between $N = 3$ and $N = \infty$. When $N \to \infty$, α_N is zero as the TP_N approximation tends to the exact solution in that case. Because the P_1 approximation, unlike all other higher order approximations, does not have a transient component, $\alpha_1(c)$ is left out in this interpolation. Hence $\alpha_N(c)$ is obtained as,

$$\alpha_N(c) = \frac{3}{N}\,\alpha_3(c), \quad N \geq 3 \tag{2.44}$$

2.5 Applications:

The TP_N approximation is now applied for the following neutron transport problems: the emergent angular flux distribution and leakage for source-free Milne-problem, the scalar flux for source-free Milne problem in case of $c = 1$, the leakage in constant source Milne problem, the critical thickness for a slab and the disadvantage factor for a fuel-moderator cell. Amongst the problems considered, the source-free Milne problem defines the

Table 2.1: Values of α_N as a function of c.

c	TP_1	TP_3
0.0	-0.442695	-0.522112
0.2	-0.436811	-0.514121
0.4	-0.375026	-0.483447
0.6	-0.273996	-0.295818
0.8	-0.182374	-0.076254
1.0	-0.103929	-0.036359
1.2	-0.036402	-0.058201
1.4	0.023245	-0.069446
1.6	0.076578	-0.063707
1.8	0.125768	-0.044994
2.0	0.171308	-0.018549

parameter $\alpha_N(c)$ by exactness of asymptotic flux; while other problems, which do not lead to the definition of the parameter, are considered to check the usefulness of the present formulation.

2.5.1 Emergent Angular Distribution $\psi(0,\mu)$ for Source-free Milne Problem:

By putting x = 0 in eqn. (2.22), $\psi(0, \mu)$ is

$$\psi(0, \mu) = a_{0+}\, \phi_{0+}(\mu) + \phi_{0-}(\mu) + \sum_j{}' A_j^{(N)} \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \qquad (2.45)$$

For TP_1 approximation, as is obvious, the emergent distribution will be due to the contribution of exact asymptotic flux. It is given by,

$$\psi(0, \mu) = a_{0+}\, \phi_{0+}(\mu) + \phi_{0-}(\mu) \qquad (2.46)$$

In the TP_3 case, for a source-free Milne problem the asymptotic coefficient is, by definition, equal to the exact value a_{0+} and the only unknown coefficient to be determined is $A_1^{(3)}$. This can be evaluated from equation (2.26b) with N = 3. Thus we get,

$$c\nu_0 \int_0^1 \frac{P_3(\mu)}{(\nu_0+\mu)}\, d\mu + a_{0+}\, c\nu_0 \int_0^1 \frac{P_3(\mu)}{(\nu_0-\mu)}\, d\mu$$

$$+ A_1^{(3)} \sum_{n=0}^{3} (2n+1)\, g_n(\nu_1) \int_0^1 P_3(\mu)\, P_n(\mu)\, d\mu = 0$$

By simplification, $A_1^{(3)}$ is given as

$$\beta_{23}(\nu_1)\, A_1^{(3)} = -\frac{c\nu_o}{4}\left[a_{o+}\left(5I_-^{(3)} - 3I_-^{(1)}\right) + \left(5I_+^{(3)} - 3I_+^{(1)}\right)\right] \qquad (2.47)$$

and the emergent distribution is

$$\psi(0, \mu) = a_{o+}\, \phi_{o+}(\mu) + \phi_{o-}(\mu) + A_1^{(3)} \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(\nu_1)\, P_n(\mu) \qquad (2.48)$$

The exact angular distribution is [5]

$$\psi(0, \mu) = c\nu_o^2 \frac{X(-\nu_o)}{(\nu_o^2 - \mu^2)X(\mu)}$$

$X(-\nu_o)$ is determined by solving the following two equations,

$$X(\nu_o)\, X(-\nu_o) = \frac{1}{2(1-c)} \frac{\nu_o^2(1-c) - 1}{\nu_o^2(\nu_o^2 - 1)}$$

and

$$\frac{X(-\nu_o)}{X(\nu_o)} = a_{o+}$$

i.e., $$X(-\nu_o) = \left\{\frac{a_{o+}}{2(1-c)} \frac{\nu_o^2(1-c) - 1}{\nu_o^2(\nu_o^2 - 1)}\right\}^{\frac{1}{2}}$$

In the conventional P_N approximation, the emergent distribution is given by,

$$\psi(0,\ \mu) = \sum_j{}' a_j^{(N)} \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j)\, P_n(\mu)$$

$$+ \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(-\nu_o^{(N)})\, P_n(\mu)$$

where $\nu_o^{(N)}$ is P_N-approximation asymptotic root. The coefficients $a_j^{(N)}$ are determined from the usual Marshak boundary conditions described by eqn.(2.24). For P_1 approximation, this gives,

$$\int_o^1 a_o^{(1)}\ \mu\ \left(\frac{1}{2} + \frac{3}{2}\,\mu\, g_1\ (\nu_o^{(1)})\right) d\mu$$

$$+ \int_o^1 \mu\ \left(\frac{1}{2} - \frac{3}{2}\,\mu\, g_1\ (\nu_o^{(1)})\right) d\mu = 0$$

or, $$a_o^{(1)} \left(\frac{1}{4} + \frac{1}{2}\, g_1\ (\nu_o^{(1)})\right) = -\left(\frac{1}{4} - \frac{1}{2}\, g_1\ (\nu_o^{(1)})\right)$$

i.e., $$a_o^{(1)} = -\frac{\frac{1}{2} - g_1(\nu_o^{(1)})}{\frac{1}{2} + g_1(\nu_o^{(1)})}$$

$\nu_o^{(1)}$ is the positive root of $g_2(\nu) = 0$, with $g_2(\nu)$ given by (2.11). Thus,

$$\nu_o^{(1)} = \frac{1}{\sqrt{3(1-c)}}$$

By use of $g_1(\nu) = \nu(1-c)$, $a_{o+}^{(1)}$ then becomes

$$a_o^{(1)} = -\frac{\frac{1}{2} - \sqrt{\frac{1-c}{3}}}{\frac{1}{2} + \sqrt{\frac{1-c}{3}}} \qquad (2.49)$$

[illegible]
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With $a_o^{(1)}$ determined from eqn. (2.49), the emergent distribution for P_1 approximation is then,

$$\psi(0,\ \mu) = a_o^{(1)} \sum_{n=o}^{1} \left(\frac{2n+1}{2}\right) g_n(\nu_o^{(1)})\ P_n(\mu)$$

$$+ \sum_{n=o}^{1} \left(\frac{2n+1}{2}\right) g_n(-\nu_o^{(1)})\ P_n(\mu) \qquad (2.50)$$

In P_3 approximation, the two coefficients $a_o^{(3)}$ and $a_1^{(3)}$ are obtained by the following conditions,

$$\int_o^1 P_1(\mu)\ \{ \sum_{j=o}^{1} a_j^{(3)} \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(\nu_j)\ P_n(\mu)$$

$$+ \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n\ (-\nu_o^{(3)})\ P_n(\mu) \}\ d\mu = 0$$

and,

$$\int_o^1 P_3(\mu)\ \{ \sum_{j=o}^{1} a_j^{(3)} \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(\nu_j)\ P_n(\mu)$$

$$+ \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n\ (-\nu_o^{(3)})\ P_n(\mu) \}\ d\mu = 0$$

Simplification of these equations yields,

$$a_o^{(3)}\ \beta_{12}(\nu_o^{(3)}) + a_1^{(3)}\ \beta_{12}(\nu_1) = -\ \beta_{12}(-\nu_o^{(3)})$$

and,

$$a_o^{(3)}\ \beta_{23}(\nu_o^{(3)}) + a_1^{(3)}\ \beta_{23}(\nu_1) = -\ \beta_{23}(-\nu_o^{(3)})$$

Solving these eqns. $a_o^{(3)}$ and $a_1^{(3)}$ are

$$a_o^{(3)} = \frac{\beta_{12}(\nu_1)\ \beta_{23}(-\nu_o^{(3)}) - \beta_{12}(-\nu_o^{(3)})\ \beta_{23}(\nu_1)}{\beta_{12}(\nu_o^{(3)})\ \beta_{23}(\nu_1) - \beta_{12}(\nu_1)\ \beta_{23}(\nu_o^{(3)})}$$

and

$$a_1^{(3)} = \frac{\beta_{23}(\nu_o^{(3)})\ \beta_{12}(-\nu_o^{(3)}) - \beta_{12}(\nu_o^{(3)})\ \beta_{23}(-\nu_o^{(3)})}{\beta_{12}(\nu_o^{(3)})\ \beta_{23}(\nu_1) - \beta_{12}(\nu_1)\ \beta_{23}(\nu_o^{(3)})}$$

where $\nu_o^{(3)}$ is the largest positive root of $g_4(\nu) = 0$, with $g_4(\nu)$ given by eqn. (2.11) and β functions already defined by eqn. (2.37). The emergent angular flux for P_3 approximation is then,

$$\psi(0,\ \mu) = \sum_{j=o}^{1} a_j^{(3)} \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(\nu_j)\ P_n(\mu)$$
$$+ \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(-\nu_o^{(3)})\ P_n(\mu) \qquad (2.51)$$

Eqns. (2.48) and (2.51) are numerically compared with exact emergent distribution and the results are tabulated in Table 2.2. It is seen that the TP_N-approximation provides significant improvements over the conventional approximation. However, the calculational results show that TP_3 is not always better than TP_1 in the range of $-1 \leq \mu \leq 0$. This is especially true for low values of c and μ nearing 0. The exact solution $\psi(0,\ \mu)$ is identically zero for $\mu > 0$. Any approximate solution will, however, produce oscillations of $\psi(0,\ \mu)$ for $0 \leq \mu \leq 1$ [44]. Of course, these oscillations

Table 2.2a: Emergent angular distribution for source-free Milne problem, c = 0.2.

μ	P_1	TP_1	P_3	TP_3	Exact
-1.0	1.2702	$0.1096\text{x}10^4$	3.4870	$0.1096\text{x}10^4$	$0.1095\text{x}10^4$
-0.9	1.1939	0.9991	2.6665	0.9943	0.9936
-0.8	1.1177	0.4998	1.9743	0.5037	0.4957
-0.7	1.0415	0.3332	1.4003	0.3416	0.3295
-0.6	0.9653	0.2499	0.9343	0.2591	0.2462
-0.5	0.8891	0.1999	0.5662	0.2068	0.1961
-0.4	0.8129	0.1666	0.2857	0.1688	0.1625
-0.3	0.7367	0.1428	0.0827	0.1385	0.1384
-0.2	0.6605	0.1249	-0.0529	0.1130	0.1200
-0.1	0.5843	0.1110	-0.1315	0.0909	0.1053
0.0	0.5081	0.0999	-0.1631	0.0718	0.0924
0.1	0.4319	0.0909	-0.1580	0.0555	
0.2	0.3556	0.0833	-0.1263	0.0421	
0.3	0.2794	0.0769	-0.7820	0.0319	
0.4	0.2032	0.0714	-0.2389	0.0254	
0.5	0.1270	0.0666	0.0264	0.0229	
0.6	0.0508	0.0624	0.0626	0.0249	
0.7	0.0254	0.0587	0.0745	0.0321	
0.8	0.1016	0.0554	0.0518	0.0449	
0.9	0.1778	0.0522	-0.0155	0.0638	
1.0	0.2540	-0.3753	-0.1377	-0.3353	

Table 2.2b: Emergent angular distribution for source-free Milne problem, c = 0.6.

μ	P_1	TP_1	P_3	TP_3	Exact
-1.0	1.0552	3.2193	1.8602	3.1451	3.2065
-0.9	0.9918	1.6168	1.5396	1.5913	1.6036
-0.8	0.9285	1.0744	1.2575	1.0795	1.0603
-0.7	0.8652	0.8011	1.0114	0.8212	0.7860
-0.6	0.8019	0.6361	0.7989	0.6578	0.6197
-0.5	0.7386	0.5254	0.6176	0.5377	0.5074
-0.4	0.6753	0.4456	0.4651	0.4400	0.4256
-0.3	0.6120	0.3851	0.3390	0.3555	0.3626
-0.2	0.5487	0.3373	0.2368	0.2800	0.3113
-0.1	0.4854	0.2983	0.1562	0.2118	0.2671
0.0	0.4221	0.2655	0.0947	0.1508	0.2225
0.1	0.3587	0.2371	0.0499	0.0977	
0.2	0.2954	0.2118	0.0194	0.0535	
0.3	0.2321	0.1885	0.0008	0.0193	
0.4	0.1688	0.1660	-0.0083	-0.0033	
0.5	0.1055	0.1433	-0.0104	-0.0133	
0.6	0.0422	0.1186	-0.0078	-0.0099	
0.7	0.0211	0.0890	-0.0030	0.0062	
0.8	0.0844	0.0481	0.0016	0.0312	
0.9	0.1477	-0.0227	0.0036	0.0487	
1.0	0.2110	-0.2146	0.0007	-0.0299	

Table 2.2c: Emergent angular distribution for source-free Milne problem, c = 0.9.

μ	P_1	TP_1	P_3	TP_3	Exact
-1.0	0.6687	0.8195	0.7420	0.7608	0.8080
-0.9	0.6286	0.7204	0.6928	0.6968	0.7081
-0.8	0.5884	0.6381	0.6388	0.6362	0.6248
-0.7	0.5483	0.5683	0.5810	0.5767	0.5539
-0.6	0.5082	0.5079	0.5205	0.5168	0.4922
-0.5	0.4680	0.4549	0.4583	0.4564	0.4375
-0.4	0.4279	0.4075	0.3955	0.3955	0.3880
-0.3	0.3878	0.3646	0.3332	0.3348	0.3424
-0.2	0.3477	0.3252	0.2725	0.2750	0.2991
-0.1	0.3076	0.2884	0.2143	0.2173	0.2564
0.0	0.2674	0.2537	0.1598	0.1627	0.2073
0.1	0.2274	0.2204	0.1100	0.1124	
0.2	0.1872	0.1879	0.0660	0.0677	
0.3	0.1471	0.1557	0.0289	0.0299	
0.4	0.1070	0.1233	-0.0004	0.0003	
0.5	0.0668	0.0902	-0.0206	-0.0200	
0.6	0.0267	0.0555	-0.0308	-0.0298	
0.7	-0.0134	0.0185	-0.0299	-0.0281	
0.8	-0.0535	-0.0218	-0.0170	-0.0142	
0.9	-0.0936	-0.0668	0.0095	0.0124	
1.0	-0.1337	-0.1186	0.0500	0.0516	

are, in general, much less in TP_N approximation when compared with the P_N-approximation. Also, TP_1 oscillation is found to be more pronounced than TP_3 case. It can be thus concluded that over the whole range of $\mu \varepsilon (-1, 1)$, TP_3 emergent distribution is better than TP_1 result. This fact will also be reflected from leakage calculation to follow in the next section.

2.5.2 Leakage for Source-free Milne Problem:

The leakage from the half space is defined as,

$$L = \int_{-1}^{1} \mu \ \psi(0, \mu) \ d\mu \qquad (2.52)$$

The numerical calculation of leakage, which is an integral parameter involving the emergent angular distribution, can also provide an overall comparison of emergent angular distribution. In conventional P_N approximation and exact treatment the contribution of the integral in eqn.(2.52) for the range of $\mu \varepsilon (0, 1)$ is zero. This follows from Marshak free-surface condition or exact boundary condition. Because of the modification of Marshak conditions, this is not so in TP_N approximation. It is to be noted that the corresponding free-surface condition in TP_N approximation is given by,

$$\int_{0}^{1} (\mu + \alpha_N) \ \psi(0, \mu) \ d\mu = 0$$

which implicitly incorporates higher order moments of angular density through α_N. Thus, the inward current from the vacuum to the medium is not zero in this case and hence the leakage in TP_N approximation is given by eqn.(2.52). The P_N leakage is given by,

$$L^{(N)} = \int_{-1}^{0} \mu \; \psi(0, \mu) \; d\mu$$

By use of eqn. (2.50) and (2.51) P_1 and P_3 leakages are

$$\begin{aligned} L^{(1)} &= a_o^{(1)} \cdot g_1(\nu_o^{(1)}) - g_1(\nu_o^{(1)}) \\ &= -g_1(\nu_o^{(1)}) \; (1-a_o^{(1)}) \qquad (2.53) \end{aligned}$$

$$\begin{aligned} L^{(3)} &= a_o^{(3)} \cdot g_1(\nu_o^{(3)}) + a_1^{(3)} \; g_1(\nu_1) - g_1(\nu_o^{(3)}) \\ &= -g_1(\nu_o^{(3)})(1-a_o^{(3)}) + a_1^{(3)} \; g_1(\nu_1) \qquad (2.54) \end{aligned}$$

For TP_1 and TP_3 approximations we get,

$$L^{(T1)} = -g_1(\nu_o)(1-a_{o+}) \qquad (2.55)$$

$$L^{(T3)} = -g_1(\nu_o)(1-a_{o+}) + A_1^{(3)} \; g_1(\nu_1^{(3)}) \qquad (2.56)$$

The exact leakage is [5]

$$L = -2\nu_o^2 \; X \; (-\nu_o) \cdot (1-c) \qquad (2.57)$$

Calculations based on eqns. (2.53)-(2.57) show that leakage improves in TP_N approximations, in general. Table 2.3 produces the results on leakage from the half-space. It is

Table 2.3: Leakage out of a source-free half space.

c	P_1	TP_1	P_3	TP_3	Exact
0.9	0.2675	0.2733	0.2779	0.2774	0.2772
0.8	0.3405	0.3611	0.3721	0.3711	0.3713
0.7	0.3874	0.4290	0.4461	0.4447	0.4466
0.6	0.4221	0.4915	0.5126	0.5113	0.5170
0.5	0.4495	0.5552	0.5754	0.5764	0.5881
0.4	0.4721	0.6254	0.6365	0.6444	0.6627
0.3	0.4914	0.7066	0.6964	0.7206	0.7427
0.2	0.5081	0.8004	0.7558	0.8092	0.8266

to be noted that TP_3 leakage is always better than TP_1 leakage values in spite of the fact that TP_3 emergent distribution may not be better than TP_1 result for $-1 \leq \mu \leq 0$. This proves the fact TP_3 oscillations of $\psi(0, \mu)$ for $\mu > 0$ is much less than TP_1 oscillations. This is observed in numerical calculation of $\Psi(0, \mu)$ as shown in Table 2.2.

2.5.3 Scalar Flux for c = 1:

Earlier calculations on source-free Milne problem have been done for $c < 1$. The special case $c = 1$ needs to be treated separately as demonstrated in the evaluation of $\alpha_N(c)$ for $c = 1$. As a check on the usefulness of TP_N approximation scheme in this case, the scalar flux $\phi(x)$ calculated for P_N and TP_N approximations is compared with the exact values. By integrating eqn. (2.38) with respect to μ over $(-1, 1)$ we get for TP_N approximation,

$$\phi(x) = z_o(1) + x + \sum_j{}' A_j^{(N)} e^{-x/\nu_j} \tag{2.58}$$

In source-free Milne problem, the use of exact value of $z_o = 0.7104$ ensures exact asymptotic flux for the case of $c = 1$. The coefficients $A_j^{(N)}$ are evaluated from eqns. (2.25b) as usual. For conventional P_N-approximation, the scalar flux is given by,

$$\phi(x) = z_o^{(N)} + x + \sum_j{}' a_j^{(N)} e^{-x/\nu_j} \tag{2.59}$$

$z_o^{(N)}$ and $a_j^{(N)}$ are determined by the usual Marshak boundary conditions (2.24). For example, the P_1 approximation $z_o^{(1)}$ is evaluated (there is no $a_j^{(N)}$ in this case) with the help of eqn. (2.24) as,

$$\int_o^1 \mu \, [- \tfrac{1}{2} \mu + \tfrac{1}{2} z_o^{(1)}] \, d\mu \quad = \quad 0$$

or $$z_o^{(1)} \quad = \quad \frac{2}{3} \quad = \quad 0.6667$$

By use of first two Marshak boundary conditions, $z_o^{(3)}$ and $a_1^{(3)}$ in P_3-approximation can be determined. $z_o^{(3)}$ is found to be equal to 0.7051. Similar calculation yields the coefficients for P_5 approximation. The exact scalar flux is given by

$$\phi(x) \quad = \quad x + z_o + \int_{-1}^{1} A(\nu) \, e^{-x/\nu} d\nu \qquad (2.60)$$

Mark [45] has evaluated the transient integral numerically and the present exact results are taken from his calculations. Table 2.4 compares the approximate solutions given by eqns. (2.58) and (2.59) with the exact results. TP_1 scalar flux is superior to P_1 flux for large values of x. TP_3 improves P_3 calculations for all but very small values of x and is nearly as accurate as P_5 results for all values of x consideredhere. This proves that a single transient term in TP_3 approximation gives fairly accurate transient

Table 2.4: Milne problem scalar flux for c = 1.

x	P_1	TP_1	P_3	TP_3	P_5	Exact
0.0	0.6667	0.7104	0.6023	0.6072	0.6108	0.5773
0.2	0.8667	0.9104	0.8360	0.8408	0.8502	0.8495
0.4	1.0667	1.1104	1.0585	1.0635	1.0725	1.0731
0.6	1.2667	1.3104	1.2737	1.2788	1.2853	1.2858
0.8	1.4667	1.5104	1.4839	1.4891	1.4930	1.4935
1.0	1.6667	1.7104	1.6908	1.6960	1.6977	1.6985
1.5	2.1667	2.2104	2.1998	2.2050	2.2035	2.2051
2.0	2.6667	2.7104	2.7031	2.7084	2.7058	2.7079

flux representation in this case. It is observed, in general, that TP_N is superior to its P_N counterpart for large x. The reason for this in obvious; while TP_N approximation, through α-formulation, constructs an exact asymptotic flux in this case, the P_N approximation is a total theory (not asymptotic and transient separately).

2.5.4 Constant Source Milne Problem:

As has been pointed out earlier, this problem explicitly uses the value of α_N in TP_N calculation. The exact angular flux in this case is [5]

$$\psi(x, \mu) = \frac{q_o}{(1-c)} + a_{o+} e^{-x/\nu_o} \phi_{o+}(\mu) + \int_0^1 A(\nu) e^{-x/\nu} \phi_\nu(\mu) \, d\nu \qquad (2.61)$$

where,

$$a_{o+} = \frac{2q_o}{(1-c)\, c\nu_o\, X(\nu_o)}$$

$$A(\nu) = -q_o(\nu_o + \nu)\, X(-\nu)\, g(c, \nu)$$

$$g(c, \nu) = \left[(1-c\nu \tanh^{-1} \nu)^2 + \frac{\pi^2 c^2 \nu^2}{4} \right]^{-1}$$

and q_o is a constant isotropic source.

The exact leakage is computed from

$$L = \int_{-1}^{0} \mu\, \psi(0, \mu)\, d\mu$$

where $\psi(0, \mu)$ is obtained from equation (2.61). This gives,

$$L = \frac{2q_o}{c} (\nu_o - I(c)),$$

where,

$$I(c) = \frac{c}{2} \int_{o}^{1} [1 + \frac{c\mu^2}{(1-\mu^2)}]\, \mu g(c, \mu)\, d\mu$$

Values of $I(c)$ are tabulated by Case, de Hoffmann and Placzek [23]. The angular flux in P_N approximation is

$$\psi(x, \mu) = \frac{q_o}{(1-c)} + \sum_j{}' a_j^{(N)} e^{-x/\nu_j}$$

$$\times \sum_{n=o}^{N} (\frac{2n+1}{2})\, g_n(\nu_j)\, P_n(\mu)$$

In this case, coefficients $a_j^{(N)}$ are determined by usual Marshak boundary conditions (2.24). Thus for P_1 approximation we get,

$$\int_{o}^{1} \mu\, (\frac{q_o}{(1-c)} + a_o^{(1)} \sum_{n=o}^{1} \frac{2n+1}{2}\, g_n(\nu_o^{(1)})\, P_n(\mu))\, d\mu = 0$$

or, $$\frac{q_o}{1-c}\, \frac{1}{2} + a_o^{(1)} [\, \frac{1}{4} + \frac{1}{2}\, g_1(\nu_o^{(1)})] = 0$$

i.e. $$a_o^{(1)} = \{ \frac{q_o}{(1-c)} \} / [\, \frac{1}{2} + g_1(\nu_o^{(1)})]$$

For P_3 approximation one gets,

$$a_o^{(3)} = \frac{q_o}{2(1-c)} \frac{\frac{1}{4}\,\beta_{12}(\nu_1) + \beta_{23}(\nu_1)}{\beta_{12}(\nu_1)\,\beta_{23}(\nu_o^{(3)}) - \beta_{12}(\nu_o^{(3)})\,\beta_{23}(\nu_1)} \tag{2.62}$$

and

$$a_1^{(3)} = -\frac{q_o}{2(1-c)} \frac{\frac{1}{4}\,\beta_{12}(\nu_o^{(3)}) + \beta_{23}(\nu_o^{(3)})}{\beta_{12}(\nu_1)\,\beta_{23}(\nu_o^{(3)}) - \beta_{12}(\nu_o^{(3)})\beta_{23}(\nu_1)} \tag{2.63}$$

where β_{mn} are defined by equation (2.37).

The TP_N flux is given as

$$\psi(x,\mu) = \frac{q_o}{(1-c)} + a_{o+}^{(N)}\, e^{-x/\nu_o}\, \phi_{o+}(\mu) + \sum_j{}' A_j^{(N)}\, e^{-x/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j)P_n(\mu)$$

In this case, it is to be noted that the asymptotic coefficient $a_{o+}^{(N)}$ is not equal to the exact asymptotic coefficient (equality holds for only source-free Milne problem on which the formulation of α_N is based). Applying the modified free-surface boundary condition for TP_1, one gets

$$\int_o^1 (\mu + \alpha_1)\left[\frac{q_o}{(1-c)} + a_{o+}^{(1)}\, \phi_{o+}(\mu)\right] d\mu = 0$$

or,

$$\frac{q_o}{(1-c)}\,\frac{1}{2} + \alpha_1 \frac{q_o}{(1-c)} + a_{o+}^{(1)} \int_o^1 \mu \frac{c\nu_o}{2(\nu_o-\mu)}\, d\mu + a_{o+}^{(1)}\, \alpha_1 \int_o^1 \frac{c\nu_o}{2(\nu_o-\mu)}\, d\mu = 0$$

i.e., $$a_{0+}^{(1)} = - \frac{\frac{q_0}{2(1-c)}\,[1+2\alpha_1]}{\frac{c\nu_0}{2}\,[(\nu_0+\alpha_1)\ \ln \frac{\nu_0}{\nu_0-1} - 1]} \tag{2.64}$$

Similarly for TP_3 approximation $a_{0+}^{(3)}$ and $A_1^{(3)}$ are,

$$a_{0+}^{(3)} = \frac{2q_0}{c\nu_0(1-c)}\ \frac{\frac{1}{8}\,[\beta_{12}(\nu_1)+\alpha_3\beta_{31}(\nu_1)] + \beta_{23}(\nu_1)(\alpha_3+\frac{1}{2})}{\frac{1}{2}\,[\beta_{12}(\nu_1)+\alpha_3\beta_{31}(\nu_1)]\ I_{31} - \beta_{23}(\nu_1)\ I_{10}} \tag{2.65}$$

$$A_1^{(3)} = - \frac{q_0}{(1-c)}\ \frac{\frac{1}{8}\ I_{10} + I_{31}(\alpha_3 + \frac{1}{2})}{\frac{1}{2}\,[\beta_{12}(\nu_1) + \alpha_3\beta_{31}(\nu_1)]\ I_{31} - \beta_{23}(\nu_1)\ I_{10}} \tag{2.66}$$

where,

$$I_{10} = I_-^{(1)} + \alpha_3\, I_-^{(0)}$$

$$I_{31} = 5I_-^{(3)} - 3I_-^{(1)}$$

α_1 and α_3 in the above equations are obtained from eqns. (2.29) and (2.35). For TP_5 calculation, $\alpha_5(c)$ is obtained from eqn. (2.44). It is observed from numerical calculation that the asymptotic coefficient in TP_N calculation is superior to the P_N values, in general. Table 2.5 compares the values of asymptotic coefficients in TP_N approximation with exact and P_N coefficients when N = 5. With the knowledge of coefficients $a_{0+}^{(N)}$ and $A_j^{(N)}$ TP_N leakage can now be easily evaluated as follows,

Table 2.5: The asymptotic coefficient for N = 5 for a half-space of constant source strength.

c	$a_o^{(5)}$	$a_{o+}^{(5)}$	a_{o+}
0.9	-3.6485	-3.6443	-3.6447
0.8	-2.0780	-2.0723	-2.0758
0.7	-1.3677	-1.3483	-1.3550
0.6	-0.9354	-0.8929	-0.8941
0.5	-0.6494	-0.5773	-0.5505
0.4	-0.4582	-0.3633	-0.2806
0.3	-0.3309	-0.2279	-0.0896
0.2	-0.2458	-0.1480	-0.0073

TP_1 Leakage

$$L^{(T1)} = \int_{-1}^{1} \mu\psi(0, \mu)\, d\mu$$

$$= \int_{-1}^{1} \mu \left[\frac{q_o}{(1-c)} + a_{o+}^{(1)}\ \phi_{o+}(\mu)\right] d\mu$$

$$= a_{o+}^{(1)}\ g_1(\nu_o)$$

TP_N Leakage

$$L^{(TN)} = a_{o+}^{(N)} \cdot g_1(\nu_o) + \sum_{j=1,2..}' A_j^{(N)}\ g_1(\nu_j^{(N)})$$

In conventional approximation, these expressions change to

$$L^{(1)} = a_o^{(1)}\ g_1(\nu_o^{(1)})$$

and,

$$L^{(N)} = \sum_{j=1,2,..}' a_j^{(N)}\ g_1(\nu_j^{(N)})$$

Leakage values with a constant source $q = \sqrt{3}(1-c)$ for exact solution, TP_N and conventional P_N approximations are produced in Table 2.6. Numerical results show that TP_N approximation does not necessarily improve leakage for high absorption (i.e., small c) cases, The reason may be attributed to poor transient flux representation for high absorptions in TP_N approximations. Thus although the asymptotic flux is improved in TP_N approximation (Table 2.5 shows this), the advantage is suppressed by a corresponding

Table 2.6: Leakage from a half-space of constant source strength.

c	P_1	TP_1	P_3	TP_3	P_5	TP_5	Exact
0.9	0.7325	0.6968	0.7179	0.7162	0.7160	0.7153	0.7147
0.8	0.6595	0.5932	0.6416	0.6385	0.6391	0.6371	0.6372
0.7	0.6126	0.5083	0.5930	0.5862	0.5900	0.5843	0.5878
0.6	0.5779	0.4254	0.5573	0.5467	0.5540	0.5400	0.5513
0.5	0.5505	0.3376	0.5291	0.5250	0.5255	0.4985	0.5227
0.4	0.5279	0.2447	0.5060	0.5518	0.5021	0.4612	0.4990
0.3	0.5086	0.1593	0.4864	0.6950	0.4823	0.4313	0.4791
0.2	0.4918	0.1154	0.4694	0.9323	0.4652	0.4097	0.4616

worsening of the transient flux for low values of c. Since leakage is an integral parameter involving angular flux, this fact is reflected in the leakage results. The failure of TP_N-approximation for small values of c in this case calls for a better transient flux representation in the approximation scheme. However, it is felt that this may not be realized in the framework of P_N approximation and a different representation for the transients may be necessary to achieve any tangible result. The other possible remedy may be to separate two class of transport problems [46] - one more close to source-free Milne problem and the other reasonably approximate to constant source Milne problem. In that case, TP_N approximation needs to be formulated separately for constant source type problems. A detailed discussion along these lines has been given in Chapter IV.

2.5.5 Critical Problem:

The present set of calculations involving a free-surface culminates in the study of critical problem in slab geometry. The exact free surface condition for a slab of half-thickness b_c is [5]

$$e^{b_c/\nu_0}\,\phi_{0+}(\mu) + e^{-b_c/\nu_0}\,\phi_{0-}(\mu) + \int_0^1 A(\nu)[e^{b_c/\nu}\,\phi_\nu(\mu) + e^{-b_c/\nu}\,\phi_{-\nu}(\mu)]\,d\nu = 0 \qquad \mu \geq 0 \qquad (2.67)$$

Eqn. (2.67) is the starting equation from which the critical half-thickness and corresponding flux distribution are determined in exact analysis. In conventional P_N approximation the free-surface condition is

$$
\begin{aligned}
& e^{b_c/\nu_o^{(N)}} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_o^{(N)})\, P_n(\mu) + \\
& + e^{-b_c/\nu_o^{(N)}} \sum_{n=o}^{N} (-1)^n \left(\frac{2n+1}{2}\right) g_n(\nu_o^{(N)})\, P_n(\mu) \\
& + \sum_j{}' a_j^{(N)} \Big[e^{b_c/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j)\, P_n(\mu) \\
& + e^{-b_c/\nu_j} \sum_{n=o}^{N} (-1)^n \frac{2n+1}{2} g_n(\nu_j)\, P_n(\mu) \Big] = 0
\end{aligned}
$$

$$\mu \geq 0 \qquad (2.68a)$$

The corresponding TP_N free-surface condition is

$$
\begin{aligned}
& e^{b_c/\nu_o} \phi_{o+}(\mu) + e^{-b_c/\nu_o} \phi_{o-}(\mu) \\
& + \sum_{j=\text{roots}}{}' A_j^{(N)} \Big[e^{b_c/\nu_j} \sum_{n=o}^{N} \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \\
& + e^{-b_c/\nu_j} \sum_{n=o}^{N} (-1)^n \left(\frac{2n+1}{2}\right) g_n(\nu_j) P_n(\mu) \Big] = 0
\end{aligned}
$$

$$\mu \geq 0 \qquad (2.68b)$$

Because of the homogeneous nature of eqns.(2.67) and (2.68) asymptotic coefficient has been put equal to unity by normalization. In eqn. (2.68a) the unknowns $\{b, a_j^{(N)}\}$

are determined by application of conventional Marshak boundary conditions while the modified free-surface conditions as given in eqn. (2.25) are used to evaluate the unknown coefficients of eqn.(2.68b). For P_1 approximation, one gets for the critical thickness $b_c^{(1)}$

$$\int_0^1 \mu \, [e^{b_c/\nu_0^{(1)}} \sum_{n=0}^{1} (\frac{2n+1}{2}) \, g_n(\nu_0^{(1)}) \, P_n(\mu)$$

$$+ e^{-b_c/\nu_0^{(1)}} \sum_{n=0}^{1} (-1)^n \, (\frac{2n+1}{2}) \, g_n(\nu_0^{(1)}) P_n(\mu)] \, d\mu = 0$$

or,
$$e^{b_c/\nu_0^{(1)}} \, [\frac{1}{4} + \frac{1}{2} g_1(\nu_0^{(1)})] + e^{-b_c/\nu_0^{(1)}} \, [\frac{1}{4} - \frac{1}{2} g_1(\nu_0^{(1)})] - = 0$$

By use of $\nu_0 = ik_0$ and noting that

$$e^{b_c/\nu_0^{(1)}} = \cos \frac{b_c}{k_0} - i \sin \frac{b_c}{k_0} ,$$

We get,

$$\frac{1}{2} \cos \frac{b_c}{k_0^{(1)}} + k_0^{(1)}(1-c) \sin \frac{b_c}{k_0^{(1)}} = 0$$

or
$$b_c^{(1)} = k_0^{(1)} \tan^{-1} (\frac{k_0^{(1)}}{\lambda^{(1)}})$$

where $k_0^{(1)} = 1/\sqrt{3(c-1)}$ and P_1 linear extrapolation length, $\lambda^{(1)} = 2/3$.

Similarly, the critical half-thickness for TP_1 approximation is obtained from the equation

$$\int_0^1 (\mu + \alpha_1) [e^{b_c/\nu_0} \phi_{0+}(\mu) + e^{-b_c/\nu_0} \phi_{0-}(\mu)] \, d\mu = 0 \tag{2.70}$$

By use of $\nu_0 = ik_0$, the expression

$$e^{b_c/\nu_0} \phi_{0+}(\mu) + e^{-b_c/\nu_0} \phi_{0-}(\mu)$$

simplifies to

$$\frac{ck_0^2}{k_0^2 + \mu^2} \cos \frac{b_c}{k_0} - \frac{ck_0\mu}{k_0^2 + \mu^2} \sin \frac{b_c}{k_0}$$

Then the condition (2.70) is written as

$$\int_0^1 (\mu+\alpha_1) \left(\frac{ck_0^2}{k_0^2+\mu^2} \cos \frac{b_c}{k_0} - \frac{ck_0\mu}{k_0^2 + \mu^2} \sin \frac{b_c}{k_0}\right) d\mu = 0$$

By use of α_1 from eqn.(2.30) it follows,

$$k_0 \tan \frac{b_c}{k_0} = \frac{k_0^2}{\lambda}$$

i.e., $$b_c^{(T1)} = k_0 \tan^{-1} (k_0/\lambda) \tag{2.71}$$

which is the end-point result [5]. Eqn.(2.71) clearly shows that replacement of different P_N-approximation parameters like $\nu_0^{(N)}$, $\lambda^{(N)}$, $z_0^{(N)}$, by their exact values (ν_0, λ, z_0) is indeed possible by a modification of free-surface conditions.

In TP_3-approximation, the two equations in the unknowns b_c and $A_1^{(3)}$ are

$$\int_0^1 (\mu+\alpha_3) \{ e^{b_c/\nu_0} \phi_{0+}(\mu) + e^{-b_c/\nu_0} \phi_{0-}(\mu) + A_1^{(3)} [e^{b_c/\nu_1} \sum_{n=0}^{3} (\frac{2n+1}{2}) g_n(\nu_1) P_n(\mu) + e^{-b_c/\nu_1} \sum_{n=0}^{3} (-1)^n (\frac{2n+1}{2}) g_n(\nu_1) P_n(\mu)] \} d\mu = 0 \qquad (2.72)$$

and,

$$\int_0^1 P_3(\mu) \{ e^{b_c/\nu_0} \phi_{0+}(\mu) + e^{-b_c/\nu_0} \phi_{0-}(\mu)\} d\mu + A_1^{(3)} [e^{b_c/\nu_1} \sum_{n=0}^{3} (\frac{2n+1}{2}) g_n(\nu_1) \int_0^1 P_n(\mu) P_3(\mu) d\mu + e^{-b_c/\nu_1} \sum_{n=0}^{3} (-1)^n (\frac{2n+1}{2}) g_n(\nu_1) \int_0^1 P_n(\mu) P_3(\mu) d\mu] = 0 \qquad (2.73)$$

We already have,

$$e^{b_c/\nu_0} \phi_{0+}(\mu) + e^{-b_c/\nu_0} \phi_{0-}(\mu) = \frac{ck_0^2}{k_0^2 + \mu^2} \cos \frac{b_c}{k_0} - \frac{ck_0\mu}{k_0^2+\mu^2} \sin \frac{b_c}{k_0}$$

The integrals of the type

$$\int_0^1 \frac{\mu^n}{(k_0^2 + \mu^2)} d\mu$$

are evaluated by the following recurrence relation [43]

$$J(n) = \int_0^1 \frac{\mu^n}{(k_o^2 + \mu^2)} \, d\mu = \frac{1}{n-1} - k_o^2 \; J(n-2)$$

with, $J(0) = \frac{1}{k_o} \tan^{-1} \left(\frac{1}{k_o}\right)$ and $J(1) = \frac{1}{2} \ln \frac{k_o^2+1}{k_o^2}$

Thus, eqn. (2.72) and (2.73) simplify to

$$\cos \frac{b_c}{k_o} [c k_o^2 \; J(1) + \alpha_3 \; c k_o^2 \; J(0)]$$

$$- \sin \frac{b_c}{k_o} [c k_o \; J(2) + c k_o \; \alpha_3 J(1)]$$

$$+ A_1^{(3)} [e^{b_c/\nu_1} \beta_{12} (\nu_1) + e^{-b_c/\nu_1} \beta_{12}(-\nu_1)$$

$$+ \alpha_3 \; e^{b_c/\nu_1} \beta_{13}(\nu_1) + \alpha_3 \; e^{-b_c/\nu_1} \beta_{13}(-\nu_1)] = 0 \qquad (2.74)$$

and,

$$c k_o^2 \cos \frac{b_c}{k_o} [\tfrac{5}{2} J(3) - \tfrac{3}{2} J(1)]$$

$$- c k_o \sin \frac{b_c}{k_o} (\tfrac{5}{2} J(4) - \tfrac{3}{2} J(2))$$

$$+ A_1^{(3)} [e^{b_c/\nu_1} \beta_{23}(\nu_1) + e^{-b_c/\nu_1} \beta_{23}(-\nu_1)] = 0 \qquad (2.75)$$

where β_{mn} are given by eqn. (2.37). Eqn. (2.74) and (2.75) are two homogeneous eqns. involving b_c and $A_1^{(3)}$. Eliminating $A_1^{(3)}$ from these equations it follows,

$$\begin{aligned}
&\{\cos \frac{b_c}{k_o}\, ck_o^2\, J(1) + ck_o^2\, \alpha_3 J(0) - \sin \frac{b_c}{k_o}\, ck_o\, J(2) \\
&\quad - ck_o \sin \frac{b_c}{k_o}\, \alpha_3 J(1)\}\{ e^{b_c/\nu_1}\, \beta_{23}(\nu_1) + e^{-b_c/\nu_1}\, \beta_{23}(-\nu_1)\} \\
&\quad - \{ ck_o^2 \cos \frac{b_c}{k_o}\, (\tfrac{5}{2}\, J(3) - \tfrac{3}{2}\, J(1)) - ck_o \sin \frac{b_c}{k_o}(\tfrac{5}{2}\, J(4) - \tfrac{3}{2} J(2))\} \\
&\qquad \{e^{b_c/\nu_1}\, \beta_{12}(\nu_1) + e^{-b_c/\nu_1}\, \beta_{12}(-\nu_1) \\
&\quad + \alpha_3\, [e^{b_c/\nu_1}\, \beta_{13}(\nu_1) + e^{-b_c/\nu_1}\, \beta_{13}(-\nu_1)] \quad = \quad 0 \qquad (2.76)
\end{aligned}$$

The solution of this transcendental equation gives the critical half thickness b_c for TP_3 approximation. For the solution of (2.76), Newton-Raphson method in employed. $\alpha_3(c)$ in obtained from eqn. (2.36). The critical half-thickness for P_3 approximation is obtained by solving a similar transcendental equation. Table 2.7 gives the critical half-thicknesses which show that the TP_3 approximation improves the end-point result (i.e. TP_1 result) further.

2.5.6 Interface Problem:

For an analysis of interface problem by TP_N method, the two half-space Milne problem is considered as the standard reference problem. The angular flux $\psi(x, \mu)$ of the two half-space Milne problem satisfies the following equation.

Table 2.7: Critical half-thickness b_c in units of mean free path.

c	P_1	TP_1	P_3	TP_3	Exact
1.02	5.7519	5.6655	5.6711	5.6655	5.6655
1.05	3.4034	3.3002	3.3066	3.3002	3.3002
1.10	2.2287	2.1134	2.1213	2.1134	2.1134
1.20	1.4125	1.2898	1.3020	1.2895	1.2893
1.40	0.8581	0.7384	0.7577	0.7364	0.7366
1.60	0.6269	0.5152	0.5384	0.5113	0.5120
1.80	0.4965	0.3932	0.4182	0.3882	0.3887
2.00	0.4121	0.3163	0.3421	0.3110	0.3108

$$\mu \frac{\partial\psi}{\partial x}(x, \mu) + \psi(x, \mu) = \frac{c}{2}\int_{-1}^{1} \psi(x, \mu')\, d\mu' \qquad x < 0$$

$$= \frac{\bar{c}}{2}\int_{-1}^{1} \psi(x, \mu')\, d\mu' \qquad x > 0 \tag{2.77}$$

with the following boundary conditions

$$\lim_{x \to \infty} \psi(x, \mu) \rightarrow e^{x/\nu_0} \phi_{0-}(\mu)$$

$$\lim_{x \to -\infty} \psi(x, \mu) = 0$$

and the interface condition

$$\psi(0+, \mu) = \psi(0-, \mu)$$

where c and $\bar{c}$ are number of secondaries per primary for the left hand and right hand media respectively.

The exact solution of eqn. (2.77) is [5]

$$\psi(x, \mu) = -a_{0-} e^{x/\nu_0} \phi_{0-}(\mu) - \int_{-1}^{0} A(\nu)\, e^{-x/\nu} \phi_\nu(\mu)\, d\nu \qquad x < 0 \tag{2.78a}$$

and,

$$\bar{\psi}(x, \mu) = e^{x/\bar{\nu}_0} \bar{\phi}_{0-}(\mu) + \bar{a}_{0+} e^{-x/\bar{\nu}_0} \bar{\phi}_{0+}(\mu) + \int_{0}^{1} A(\nu)\, e^{-x/\nu} \bar{\phi}_\nu(\mu)\, d\nu, \quad x > 0 \tag{2.78b}$$

The coefficients a_{0-}, $\bar{a}_{0+}$ and $A(\nu)$ are given as [5]

$$\bar{a}_{0+} = \frac{\chi(-\bar{\nu}_0)\,(\nu_0 - \bar{\nu}_0)}{\chi(\bar{\nu}_0)\,(\nu_0 + \bar{\nu}_0)}$$

$$a_{0-} = \frac{\chi(-\bar{\nu}_0)}{\chi(-\nu_0)} \cdot \frac{2\,\bar{c}\;\bar{\nu}_0^2}{c\nu_0\,(\nu_0 + \bar{\nu}_0)}$$

$$A(\nu) = -\frac{\nu\bar{c}(1-\bar{c})\,\bar{\nu}_0^2\,(\nu_0 - \bar{\nu}_0)\,\chi(-\bar{\nu}_0)\,\bar{X}(-\nu)}{(\nu_0 + \nu)\,\bar{N}(\nu)\,X(-\nu)}, \quad \nu > 0$$

$$A(\nu) = -\frac{\nu\bar{c}(1-c)\,\bar{\nu}_0^2\,(\nu_0 - \bar{\nu}_0)\,\chi(-\bar{\nu}_0)\,X(\nu)(\nu_0 - \nu)}{(\bar{\nu}_0^2 - \nu^2)\,N(\nu)\,\bar{X}(\nu)}, \quad \nu < 0$$

where, χ- function is defined as

$$\chi(Z) = \bar{X}(Z)\,X(-z)$$

and,

$$N(\nu) = \frac{\nu}{g(c,\,\nu)}$$

X and g-functions in these equations have already been defined. In the TP_N formalism, the solution (2.78) becomes,

$$\psi(x,\,\mu) = -a_{0-}^{(N)}\,e^{x/\nu_0}\,\phi_{0-}(\mu) - \sum_j{}' A_j^{(N)}\,e^{x/\nu_j} \times \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(-\nu_j)\,P_n(\mu), \quad x < 0 \qquad (2.79a)$$

and,

$$\bar{\psi}(x,\,\mu) = e^{x/\bar{\nu}_0}\,\bar{\phi}_{0-}(\mu) + \bar{a}_{0+}^{(N)}\,e^{-x/\bar{\nu}_0}\,\bar{\phi}_{0+}(\mu) + \sum_j{}' \bar{A}_j^{(N)}\,e^{-x/\bar{\nu}_j} \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) g_n(\bar{\nu}_j)\,P_n(\mu), \quad x > 0 \qquad (2.79b)$$

where prime in the j-summation indicates that only positive roots are taken. The interface condition then is

$$-a_{0-}^{(N)} \phi_{0-}(\mu) - \sum_j{}' A_j^{(N)} \sum_{n=0}^{N} (\frac{2n+1}{2})\, g_n(-\nu_j)\, P_n(\mu)$$

$$= \bar{\phi}_{0-}(\mu) + \bar{a}_{0+}^{(N)} \bar{\phi}_{0+}(\mu) + \sum_j{}' \bar{A}_j^{(N)} \sum_{n=0}^{N} (\frac{2n+1}{2})\, g_n(\bar{\nu}_j) P_n(\mu) \qquad (2.80)$$

Multiplying both sides of eqn.(2.80) by $P_n(\mu)$ and integrating with respect to μ between -1 and 1, it follows

$$-a_{0-}^{(N)} g_n(-\nu_0) - \sum_j{}' A_j^{(N)} g_n(-\nu_j)$$

$$= g_n(-\bar{\nu}_0) + \bar{a}_{0+}^{(N)} g_n(\bar{\nu}_0) + \sum_j{}' \bar{A}_j^{(N)} g_n(\bar{\nu}_j) \quad \ldots$$

$$n = 0,1,2,..N \qquad (2.81)$$

Eqn. (2.81) is just of the same form as the interface condition used in conventional P_N approximation. In TP_N approximation, we wish to have an exact transport theory asymptotic flux for the Milne problem treating the adjoining half-space as purely absorbing ($c = 0$). Thus a parameter $\delta_N(c)$ is introduced in the first equation of the set of eqns. (2.81) as

$$-a_{0-}^{(N)} - \sum_j{}' A_j^{(N)} = 1 + \delta_N \{ \bar{a}_{0+}^{(N)} + \sum_j{}' \bar{A}_j^{(N)} \} \qquad (2.82)$$

Note that $\delta_N(c)$ is introduced as a multiplying factor in the non-source part of the solution. The eqn. (2.82) alongwith the following eqns

$$-a_{o-}^{(N)} \; g_n(-\nu_o) - \sum_j{}' A_j^{(N)} \; g_n(-\nu_j)$$

$$= g_n(-\bar{\nu}_o) + \bar{a}_{o+}^{(N)} \; g_n(\bar{\nu}_o) + \sum_j{}' \bar{A}_j^{(N)} \; g_n(\bar{\nu}_j)$$

$$n = 1,2,3,\ldots N \qquad (2.83)$$

constitute the interface conditions for evaluation of the coefficients.

Determination of $\delta_N(c)$ for TP_1 and TP_3 Approximations:

$\delta_N(c)$ is determined by the condition that exact asymptotic flux be obtained for the right side medium treating the adjoining half-space as a purely absorbing one i.e. c = o. In that case, $\bar{a}_{o+}^{(N)}$ takes its exact value i.e.,

$$\bar{a}_{o+}^{(N)} = \bar{a}_{o+} = -e^{-2\bar{z}_o/\bar{\nu}_o}$$

In TP_1 approximation, it follows from eqn. (2.82),

$$-a_{o-}^{(1)} = 1 + \delta_1 \, \bar{a}_{o+} \qquad (2.84)$$

when c = 0, the asymptotic flux in the left hand side medium is zero. Therefore, we get,

$$a_{o-}^{(1)} = 0$$

The condition (2.84) then becomes

$$1 + \delta_1 \, \bar{a}_{o+} = 0$$

i.e. $$\delta_1 = -\frac{1}{\bar{a}_{o+}} = e^{2\bar{z}_o/\bar{\nu}_o} \qquad (2.85)$$

For TP_3-approximation, from eqns. (2.82) and (2.83) the interface conditions are as follows,

$$-a_{o-}^{(3)} - A_1^{(3)} = 1 + \delta_3 \{ \bar{a}_{o+}^{(3)} + \bar{A}_1^{(3)} \}$$

$$- a_{o-}^{(3)} g_n(-\nu_o) - A_1^{(3)} g_n(-\nu_1)$$

$$= g_n(-\bar{\nu}_o) + \bar{a}_{o+}^{(3)} g_n(\bar{\nu}_o) + \bar{A}_1^{(3)} g_n(\nu_1)$$

$$n = 1,2,3$$

when $c = 0$, $a_{o-}^{(3)} = 0$ and $\bar{a}_{o+}^{(3)} = \bar{a}_{o+} = -e^{-2\bar{z}_o/\bar{\nu}_o}$

Then, δ_3 is determined from the following equations

$$-A_1^{(3)} = 1 + \delta_3 \{ \bar{a}_{o+} + \bar{A}_1^{(3)} \} \qquad (2.86)$$

$$-A_1^{(3)} g_n(-\nu_1)|_{c=o} = g_n(-\bar{\nu}_o) + \bar{a}_{o+} g_n(\bar{\nu}_o)$$

$$+ \bar{A}_1^{(3)} g_n(\bar{\nu}_1), \; n = 1,2 \qquad (2.87)$$

In eqn. (2.87), $g_n(-\nu_1)$ has to be evaluated at $c = 0$ and it is denoted as $g_n(-\nu_1)|_{c=o}$

From eqns.(2.86) and (2.87), it follows

$$\delta_3 = - \frac{1 + \dfrac{\begin{matrix} E_{R1} & E_{12} \\ E_{R2} & E_{22} \end{matrix}}{\begin{matrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{matrix}}}{\dfrac{\begin{matrix} E_{11} & E_{R1} \\ E_{21} & E_{R2} \end{matrix}}{\begin{matrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{matrix}} - e^{-2\bar{z}_o/\bar{\nu}_o}} \qquad (2.88)$$

where,

$$E_{11} = g_1(\nu_1)\Big|_{c=o} \quad , \quad E_{21} = -g_2(\nu_1)_{c=o}$$

$$E_{12} = -g_1(\bar{\nu}_1) \quad , \quad E_{22} = -g_2(\bar{\nu}_1)$$

and,

$$E_{R1} = (-e^{-2\bar{z}_o/\bar{\nu}_o} - 1) \quad g_1(\bar{\nu}_o)$$

$$E_{R2} = (-e^{-2z_o/\nu_o} + 1) \quad g_2(\bar{\nu}_o)$$

The values of δ_1 and δ_3 as obtained from eqns. (2.85) and (2.88) will be used for any problem involving interface.

Fuel-Moderator Cell Problem:

An infinite homogeneous array of 2w cm wide fuel plates separated by a moderator with a centre-line spacing of W cm is considered. The disadvantage factor 'd' in such an array is defined as the ratio of average flux in the moderator to the average flux in the fuel i.e.,

$$d = \frac{\frac{1}{W - w} \int_{w}^{W} \bar{\phi}(x)\, dx}{\frac{1}{w} \int_{0}^{w} \phi(x)\, dx} \qquad (2.89)$$

where $\phi(x)$ is the scalar flux for the fuel and $\bar{\phi}(x)$ is that for the moderator. All the quantities under the bar are used in case of moderator. The disadvantage factor 'd' will be calculated by TP_N formalism and the results will be compared with values obtained by conventional P_N approximation and exact solution.

In the TP_1 approximation, noting that angular fluxes both in the fuel and moderator regions are symmetric about their mid-plane, the angular fluxes are given as, (with the origin at the centre of the fuel)

$$\psi(x,\ \mu) \ = \ a_{o+}^{(1)} \left\{ \frac{c\nu_o}{2(\nu_o+\mu)}\, e^{\Sigma x/\nu_o} + \frac{c\nu_o}{2(\nu_o-\mu)}\, e^{-\Sigma x/\nu_o} \right\} \tag{2.90}$$

$$\bar{\psi}(x,\ \mu) \ = \ \bar{a}_{o+}^{(1)} \left\{ \frac{\bar{c}\ \bar{\nu}_o}{2(\bar{\nu}_o+\mu)}\, e^{\bar{\Sigma}(x-W)/\bar{\nu}_o} + \frac{\bar{c}\ \bar{\nu}_o}{2(\bar{\nu}_o-\mu)}\, e^{-\bar{\Sigma}(x-W)/\bar{\nu}_o} \right\} + \frac{S}{(1-\bar{c})} \tag{2.91}$$

A spatially constant source has been taken in the moderator region with no source in the fuel. The factors Σ and $\bar{\Sigma}$ are incorporated in eqns. (2.90) and (2.91) because distances in this case are measured in cms. The interface conditions at the interface $x = W$ are obtained from eqns. (2.90) and (2.91) as

$$a_{o+}^{(1)} \ \cosh \frac{\Sigma x}{\nu_o}\Big|_{x=W} \ = \ \delta_1\ \bar{a}_{o+}^{(1)} \ \cosh \frac{\bar{\Sigma}(x-W)}{\bar{\nu}_o}\Big|_{x=W} + \frac{S}{(1-\bar{c})} \tag{2.92}$$

and,

$$a_{o+}^{(1)} \ g_1(\nu_o)\ \sinh \frac{\Sigma x}{\nu_o}\Big|_{x=W} \ = \ \bar{a}_{o+}^{(1)} \ g_1(\bar{\nu}_o)\ \sinh \frac{\bar{\Sigma}(x-W)}{\bar{\nu}_o}\Big|_{x=W} \tag{2.93}$$

It is to be noted that with the introduction of the parameter δ_1, the moderator scalar flux is given by the right hand side of eqn. (2.92). Thus the scalar flux at the interface is continuous - this is at variance with Pomraning's asymptotic theory [26] or the usual asymptotic diffusion theory where a discontinuity is allowed to improve the overall result. In addition, the present formulation by its construction yields a better angular flux. $a_{0+}^{(1)}$ and $\bar{a}_{0+}^{(1)}$ are given from eqns. (2.92) and (2.93) as

$$a_{0+}^{(1)} = \frac{g_1(\bar{\nu}_0)\sinh\frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}}{(1-\bar{c})\left\{g_1(\bar{\nu}_0)\sinh\frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}\cosh\frac{\Sigma w}{\nu_0} + \delta_1 g_1(\nu_0)\sinh\frac{\Sigma w}{\nu_0}\cosh\frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}\right\}} \qquad (2.94)$$

$$\bar{a}_{0+}^{(1)} = \frac{g_1(\nu_0)\sinh\frac{\Sigma w}{\nu_0}}{(1-\bar{c})\left\{g_1(\bar{\nu}_0)\sinh\frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}\cosh\frac{\Sigma w}{\nu_0} + \delta_1 g_1(\nu_0)\sinh\frac{\Sigma w}{\nu_0}\cosh\frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}\right\}} \qquad (2.95)$$

The disadvantage factor is obtained from eqn. (2.89) as

$$d = \frac{\frac{1}{(1-\bar{c})} + \delta_1 \bar{a}_{0+}^{(1)} \frac{\bar{\nu}_0}{(W-w)\bar{\Sigma}}\sinh\frac{(W-w)\bar{\Sigma}}{\bar{\nu}_0}}{\frac{1}{w} a_{0+}^{(1)} \frac{\nu_0}{\Sigma}\sinh\frac{w\Sigma}{\nu_0}}$$

By use of $a_{o+}^{(1)}$ and $\bar{a}_{o+}^{(1)}$ from eqns. (2.94) and (2.95), this expression simplifies to

$$d = \frac{w\Sigma}{\nu_o} \coth \frac{\Sigma w}{\nu_o} + \delta_1 \frac{w}{W-w} \frac{(1-c)\Sigma}{(1-\bar{c})\bar{\Sigma}}$$

$$\times \left\{ (W-w) \frac{\bar{\Sigma}}{\bar{\nu}_o} \coth \frac{\bar{\Sigma}(W-w)}{\bar{\nu}_o} - 1 \right\} \qquad (2.96)$$

The conventional P_1-approximation disadvantage factor follows from eqn. (2.96) by replacing ν_o, $\bar{\nu}_o$ by their P_1 values and by putting $\delta_1 = 1$. Thus it follows for P_1-approximation,

$$d = \frac{w\Sigma}{\nu_o^{(1)}} \coth \frac{\Sigma w}{\nu_o^{(1)}} + \frac{w}{W-w} \frac{(1-c)\Sigma}{(1-\bar{c})\bar{\Sigma}}$$

$$\times \left\{ (W-w) \frac{\bar{\Sigma}}{\bar{\nu}_o^{(1)}} \coth \frac{\bar{\Sigma}(W-w)}{\bar{\nu}_o^{(1)}} - 1 \right\} \qquad (2.97)$$

In TP_3-approximation, the angular flux in the fuel and moderator sides are given as

$$\psi(x, \mu) = a_{o+}^{(3)} \left\{ \frac{c\nu_o}{2(\nu_o+\mu)} e^{\Sigma x/\nu_o} + \frac{c\nu_o}{2(\nu_o-\mu)} e^{-\Sigma x/\nu_o} \right\}$$

$$+ A_1^{(3)} \left\{ \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(-\nu_1) P_n(\mu) e^{\Sigma x/\nu_1} \right.$$

$$\left. + \sum_{n=o}^{3} \left(\frac{2n+1}{2}\right) g_n(\nu_1) P_n(\mu) e^{-\Sigma x/\nu_1} \right\} \qquad (2.98)$$

$$\bar{\psi}(x,\ \mu) = \bar{a}_{o+}^{(3)} \{ \frac{\bar{c}\ \bar{\nu}_o}{2(\bar{\nu}_o+\mu)} e^{\bar{\Sigma}(x-W)/\bar{\nu}_o} + \frac{\bar{c}\ \bar{\nu}_o}{2(\bar{\nu}_o-\mu)} e^{-\bar{\Sigma}(x-W)/\bar{\nu}_o} \}$$

$$+ \bar{A}_1^{(3)} \{ \sum_{n=o}^{3} (\frac{2n+1}{2})\ g_n(-\bar{\nu}_1) P_n(\mu)\ e^{\bar{\Sigma}(x-W)/\bar{\nu}_1} + \sum_{n=o}^{3} (\frac{2n+1}{2})\ g_n(\bar{\nu}_1)\ P_n(\mu)\ e^{-\bar{\Sigma}(x-W)/\bar{\nu}_1} \} + \frac{S}{(1-\bar{c})} \tag{2.99}$$

The interface conditions for TP$_3$-approximation are obtained at $x = w$ as,

$$a_{o+}^{(3)} \cosh \frac{\Sigma w}{\nu_o} + A_1^{(3)} \cosh \frac{\Sigma w}{\nu_1} = \delta_3 \{ \bar{a}_{o+}^{(3)} \cosh \frac{(W-w)\bar{\Sigma}}{\bar{\nu}_o} + \bar{A}_1^{(3)} \cosh \frac{(W-w)\bar{\Sigma}}{\bar{\nu}_1} \} + \frac{S}{(1-\bar{c})} \tag{2.100}$$

$$a_{o+}^{(3)}\ g_1(\nu_o) \sinh \frac{\Sigma w}{\nu_o} + A_1^{(3)}\ g_1(\nu_1) \operatorname{Sinh} \frac{\Sigma w}{\nu_1} = -\{ \bar{a}_{o+}^{(3)}\ g_1(\bar{\nu}_o) \sinh \frac{(W-w)\bar{\Sigma}}{\bar{\nu}_o} + \bar{A}_1^{(3)}\ g_1(\bar{\nu}_1) \sinh \frac{(W-w)\bar{\Sigma}}{\bar{\nu}_1} \} \tag{2.101}$$

$$a_{0+}^{(3)}\, g_2(\nu_0) \cosh \frac{\Sigma w}{\nu_0} + A_1^{(3)}\, g_2(\nu_1) \cosh \frac{\Sigma w}{\nu_1}$$
$$= \bar{a}_{0+}^{(3)}\, g_2(\bar{\nu}_0) \cosh \frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}$$
$$+ \bar{A}_1^{(3)}\, g_2(\bar{\nu}_1) \cosh \frac{\bar{\Sigma}(W-w)}{\nu_1} \qquad (2.102)$$

$$a_{0+}^{(3)}\, g_3(\nu_0) \sinh \frac{\Sigma w}{\nu_0} + A_1^{(3)}\, g_3(\nu_1) \sinh \frac{\Sigma w}{\nu_1}$$
$$= -\{\, \bar{a}_{0+}^{(3)}\, g_3(\bar{\nu}_0) \sinh \frac{\bar{\Sigma}(W-w)}{\bar{\nu}_0}$$
$$+ \bar{A}_1^{(3)}\, g_3(\bar{\nu}_1) \sinh \frac{\bar{\Sigma}(W-w)}{\bar{\nu}_1} \,\} \qquad (2.103)$$

Using $\delta_3(c)$ from eqn. (2.88), eqns.(2.100)-(2.103) can be solved for the coefficients $a_{0+}^{(3)}$, $\bar{a}_{0+}^{(3)}$, $A_1^{(3)}$ and $\bar{A}_1^{(3)}$. The TP_3 disadvantage factor is then calculated from eqn.(2.89). The conventional result follows by replacing the asymptotic roots by their P_3 values and by putting $\delta_3 = 1$. In order to compare the TP_N results with conventional P_N results, two fuel-moderator cells given by Murray [47] and Weinberg and Wigner [44] have been considered. The results are shown in Tables 2.8 and 2.9 respectively. It is found that TP_N approximation improves the result significantly.

Table 2.8: Cell disadvantage factor for problem 1 [47]

$w = 0.635$ cm		$W = 15.240$ cm	
$\Sigma_s = 0.3970\ \text{cm}^{-1}$		$\bar{\Sigma}_s = 0.398\ \text{cm}^{-1}$	
$\Sigma_t = 0.3748\ \text{cm}^{-1}$		$\bar{\Sigma}_t = 0.398\ \text{cm}^{-1}$	
$\Sigma_a = 3.31 \times 10^{-4}\ \text{cm}^{-1}$		$\bar{\Sigma}_a = 0.324\ \text{cm}^{-1}$	

	Disadvantage factor
P_1 theory	2.213
P_3 theory	2.405
Exact	--
TP_1 theory	2.330
TP_3 theory	2.458

Table 2.9: Cell disadvantage factor for Problem 2 [44].

w = 0.9294 cm

Σ_s = 0.3951 cm^{-1}

Σ_t = 0.3951 cm^{-1}

Σ_a = 0.3796 cm^{-1}

W = 29.3104 cm

$\bar{\Sigma}_s$ = 0.404819 cm^{-1}

$\bar{\Sigma}_t$ = 0.404819 cm^{-1}

$\bar{\Sigma}_a$ = 3.81×10^{-4} cm^{-1}

	Disadvantage factor	Percentage error
P_1 theory	5.201	5.30
P_3 theory	5.462	0.51
Exact	5.490	-
TP_1 theory	5.420	1.27
TP_3 theory	5.482	0.14

CHAPTER III

ANALYSIS OF FINITE SLAB PROBLEM

Introduction:

The work of the present chapter concerns the application of the singular eigenfunction method for monoenergetic neutron transport in a finite slab. From what has been outlined in Chapter I, it is seen that the problem of neutron transport in a finite slab reduces to the solution of two coupled Fredholm integral equations. Previous works in this area were mainly concerned with numerical solution of these integral equations. The present analysis also starts from the integral equations but differs in the important respect that the two integral equations involving the discrete and continuum coefficients are combined together to form a single Fredholm integral equation. Function analytic study of this integral eqn. is the central theme of the present chapter. For the finite slab, the critical problem is posed as an inverse eigenvalue problem where the eigenvalue is given and a parametric variation of the operator has to be determined. When the eigenvalue is unity, it defines the critical slab problem and the corresponding inverse parameter is the critical half-thickness. It is proved that the solution of finite slab critical problem is unique. A good estimate of the inverse parameter (i.e. the critical thickness) is also obtained by application of bounds of spectral radius of linear positive operators. This involves the solution of a transcendental equation which is achieved by the method of bisection. At the end of the chapter, a short discussion on uniqueness of solution of slab albedo problem is also given.

3.1 Fredholm Integral Equations of Case's Theory:

We consider neutron transport in a slab of thickness 2b which is centered at the origin. In the case of slab albedo problem, a parallel beam of neutron is incident on the surface $x = -b$, while the absence of incident neutrons defines the critical problem. Mathematical representation of the problem is given by the following equations when the scattering is isotropic

$$\mu \frac{\partial \psi}{\partial x}(x, \mu) + \psi(x, \mu) = \frac{c}{2}\int_{-1}^{1} \psi(x, \mu')\, d\mu' \quad (3.1)$$

$$\begin{aligned} \psi(-b, \mu) &= \delta(\mu-\mu_0), \quad \mu, \mu_0 > 0 \text{ for albedo problem} \\ &= 0, \quad \mu > 0 \text{ for critical problem} \\ \psi(b, \mu) &= 0 \quad \mu < 0 \end{aligned}$$

$$(3.2)$$

In Chapter II, the general solution of eqn. (3.1) is already given and discussed. In the following, we adopt the methods of McCormick and Mendelson [17] to obtain the coupled Fredholm equations referred to earlier. Thus the solution of (3.1) is written as,

$$\psi(x, \mu) = a_{0+} e^{-x/\nu_0} \phi_{0+}(\mu) + a_{0-} e^{x/\nu_0} \phi_{0-}(\mu) + \int_{-1}^{1} A(\nu) e^{-x/\nu} \phi_\nu(\mu) \, d\nu$$

where the asymptotic roots $\nu_0 \not\in (-1, 1)$ are the solution of the eqn.

$$\frac{c\nu}{2} \ln \frac{\nu+1}{\nu-1} = 1$$

and the transient roots $\nu \in (-1, 1)$. The eigenmodes $\phi_{0\pm}(\mu)$ and $\phi_\nu(\mu)$ are given by

$$\phi_{0\pm}(\mu) = \frac{c\nu_0}{2} / (\nu_0 \mp \mu)$$
$$\phi_\nu(\mu) = \frac{c\nu}{2} P \frac{1}{\nu-\mu} + \lambda(\nu) \, \delta(\nu-\mu)$$

where P denotes the principal value and $\lambda(\nu)$ is defined as

$$\lambda(\nu) = 1 - c\nu \tanh^{-1}\nu$$

To allow integration in the transient term between 0 to 1 only, the angular density $\psi(x, \mu)$ is written in the form

$$\psi(x, \mu) = a_{0+} \phi_{0+}(\mu) e^{-x/\nu_0} + a_{0-} e^{x/\nu_0} \phi_{0-}(\mu) + \int_0^1 A(\nu) \phi_\nu(\mu) e^{-x/\nu} d\nu + \int_0^1 A(-\nu) \phi_{-\nu}(\mu) e^{x/\nu} d\nu \qquad (3.3)$$

By application of boundary condition (3.2) in equation (3.3), the following equations are obtained for the coefficients $a_{0\pm}$ and $A(\nu)$.

$$\delta(\mu-\mu_0) = a_{0+}\, e^{b/\nu_0}\, \phi_{0+}(\mu) + a_{0-}\, e^{-b/\nu_0}\, \phi_{0-}(\mu) + \int_0^1 A(\nu)\, \phi_\nu(\mu)\, e^{b/\nu}\, d\nu + \int_0^1 A(-\nu)\, \phi_{-\nu}(\mu)\, e^{-b/\nu}\, d\nu, \quad \mu > 0 \qquad (3.4)$$

$$0 = a_{0+}\, e^{-b/\nu_0}\, \phi_{0+}(\mu) + a_{0-}\, e^{b/\nu_0}\, \phi_{0-}(\mu) + \int_0^1 A(\nu)\, \phi_\nu(\mu)\, e^{-b/\nu}\, d\nu + \int_0^1 A(-\nu)\, \phi_{-\nu}(\mu)\, e^{b/\nu}\, d\nu, \quad \mu < 0 \qquad (3.5)$$

Changing the variable μ to $-\mu$ in eqn. (3.5), gives,

$$0 = a_{0+}\, e^{-b/\nu_0}\, \phi_{0-}(\mu) + a_{0-}\, e^{b/\nu_0}\, \phi_{0+}(\mu) + \int_0^1 A(\nu)\, \phi_{-\nu}(\mu)\, e^{-b/\nu}\, d\nu + \int_0^1 A(-\nu)\, \phi_\nu(\mu)\, e^{b/\nu}\, d\nu, \quad \mu > 0 \qquad (3.6)$$

Adding and subtracting eqns. (3.4) and (3.6) it follows,

$$\delta(\mu-\mu_0) = \phi_{0+}(\mu)\, e^{b/\nu_0}\, (a_{0+} \pm a_{0-}) + \phi_{0-}(\mu)\, e^{-b/\nu_0}\, (a_{0-} \pm a_{0+})$$

$$+\int_0^1 (A(\nu) \pm A(-\nu))\, e^{b/\nu} \phi_\nu(\mu)\, d\nu$$

$$+\int_0^1 (A(-\nu) \pm A(\nu))\, e^{-b/\nu} \phi_{-\nu}(\mu)\, d\nu \qquad (3.7)$$

Eqn. (3.7) is rewritten as,

$$\delta(\mu-\mu_o) = b_\pm\, \phi_{o+}(\mu) \pm b_\pm\, e^{-2b/\nu_o}\, \phi_{o-}(\mu) + \int_0^1 B_\pm(\nu)\, \phi_\nu(\mu)\, d\nu \pm \int_0^1 B_\pm(\nu)\, e^{-2b/\nu}\, \phi_{-\nu}(\mu)\, d\nu, \quad \mu > 0 \qquad (3.8)$$

where the new coefficients $b_\pm$ and $B_\pm(\nu)$ are defined as

$$b_\pm = (a_{o+} \pm a_{o-})\, e^{b/\nu_o} \qquad (3.9)$$

$$B_\pm(\nu) = (A(\nu) \pm A(-\nu))\, e^{b/\nu} \qquad (3.10)$$

The coefficients $b_\pm$ and $B_\pm(\nu)$ of eqn. (3.8) are evaluated by half-range orthogonality relations. It is known that the functions $\phi_{o+}(\mu)$ and $\phi_\nu(\mu)$, $0 \leq \nu \leq 1$ form a complete set for functions defined in the range $0 \leq \mu \leq 1$. Also the functions $\phi_{o+}(\mu)$ and $\phi_\nu(\mu)$ are orthogonal with respect to a weight function $W(\mu) = \gamma(\mu)\, (\nu_o-\mu)$ where,

$$\gamma(\mu) = \frac{c}{2\,(1-c)}\; \frac{\mu}{X(-\mu)\,(\nu_o^2 - \mu^2)}$$

Thus, eqn. (3.8) is multiplied by $W(\mu).\phi_{o+}(\mu)$ and $W(\mu).\,\phi_\nu(\mu)$

and then integrated with respect to μ between 0 and 1 to obtain the following equations for evaluation of $b_{\pm}$ and $B_{\pm}(\nu)$

$$\int_0^1 \delta(\mu-\mu_o)\, W(\mu)\, \phi_{o+}(\mu)\, d\mu = b_{\pm} \int_0^1 W(\mu)\, \phi_{o+}(\mu)\, \phi_{o+}(\mu)\, d\mu$$

$$\pm\, e^{-2b/\nu_o}\, b_{\pm} \int_0^1 W(\mu)\, \phi_{o+}(\mu)\, \phi_{o-}(\mu)\, d\mu$$

$$+ \int_0^1 B_{\pm}(\nu) \int_0^1 W(\mu)\, \phi_{o+}(\mu)\, \phi_{\nu}(\mu)\, d\mu\, d\nu$$

$$\pm \int_0^1 B_{\pm}(\nu)\, e^{-2b/\nu_o} \int_0^1 W(\mu)\, \phi_{o+}(\mu)\, \phi_{-\nu}(\mu)\, d\mu\, d\nu \qquad (3.11)$$

$$\int_0^1 \delta(\mu-\mu_o)\, W(\mu)\, \phi_{\nu}(\mu)\, d\mu = b_{\pm} \int_0^1 W(\mu)\, \phi_{\nu}(\mu)\, \phi_{o+}(\mu)\, d\mu$$

$$\pm\, e^{-2b/\nu_o}\, b_{\pm} \int_0^1 W(\mu)\, \phi_{\nu}(\mu)\, \phi_{o-}(\mu)\, d\mu$$

$$+ \int_0^1 B_{\pm}(\nu') \int_0^1 W(\mu)\, \phi_{\nu'}(\mu)\, \phi_{\nu}(\mu)\, d\mu\, d\nu'$$

$$\pm \int_0^1 B_{\pm}(\nu')\, e^{-2b/\nu'} \int_0^1 W(\mu)\, \phi_{\nu}(\mu)$$

$$\times\ \phi_{-\nu'}(\mu)\, d\mu\, d\nu' \qquad (3.12)$$

Eqns.(3.11) and (3.12) simplify to

$$b_{\pm} = \left[\, \frac{2}{c}\, \gamma(\mu_o) \mp \int_0^1 B_{\pm}(\nu)\, \nu\, X(-\nu)\, e^{-2b/\nu}\, d\nu \,\right]$$

$$\times \left[\, \nu_o\, X(-\nu_o)\, \left(e^{2z_o/\nu_o} \pm e^{-2b/\nu_o}\right)\right]^{-1} \qquad (3.13)$$

$$Z_o(c) = -\frac{\nu_o}{2} \ln \left[- \frac{X(-\nu_o)}{X(\nu_o)} \right]$$

$$\gamma(\mu) = \frac{c}{2(1-c)} \quad \frac{\mu}{X(-\mu)\ (\nu_o^2 - \mu^2)},$$

$$f(c, \nu) = (1-c)\ g(c, \nu)\ X(-\nu)\ (\nu_o^2 - \nu^2)$$

and,

$$g(c, \nu) = [(1 - c\,\nu \tanh^{-1} \nu)^2 + (\tfrac{\pi c \nu}{2})^2]^{-1}$$

X(ν) is the well-known X-function of Case's theory and can be evaluated from the following eqn.

$$X(-\nu) = \exp \left[-\frac{c}{2} \int_0^1 g(c, \nu')\ \left(1 + \frac{c\,\nu'}{1-\nu'^2}\right) \ln (\nu+\nu')\ d\nu' \right] \tag{3.16}$$

Just like previous attempts on similar kinds of problems, eqns. (3.13) and (3.15) constitute the starting point of the present work. But instead of dealing the two equations separately for numerical calculation, we combine them to get a single non-homogeneous Fredholm equation for $B_\pm(\nu)$

$$\begin{aligned} B_\pm(\nu) = {} & f(c\ \nu)\Big[\frac{2}{c\,\nu}\ \gamma(\mu_o)\ \phi_\nu(\mu_o) + \gamma(\mu_o)\ h_\pm(c, \nu, b) \\ & \mp \frac{c}{2} \int_0^1 B_\pm\ (\nu')\ X(-\nu')\ e^{-2b/\nu'} \\ & \times\ \nu'\ \left(\frac{1}{\nu+\nu'} + h_\pm\ (c, \nu, b)\right)\ d\nu'\Big] \end{aligned} \tag{3.17}$$

in which

$$h_{\pm}(c,\nu,b) = \frac{\dfrac{e^{2z_0/\nu_0}}{\nu_0-\nu} \mp \dfrac{e^{-2b/\nu_0}}{\nu_0+\nu}}{e^{2z_0/\nu_0} \pm e^{-2b/\nu_0}}$$

Mathematically, the slab albedo problem is defined exclusively by eqn. (3.17). For a critical slab problem,

i) in the absence of incident neutrons, $\delta(\mu-\mu_0) \equiv 0$, and

$$\gamma(\mu_0) = \int \gamma(\mu)\ \delta(\mu-\mu_0)\ d\mu$$

is identically zero.

ii) because of the symmetry of the problem

$$a_{0+} = a_{0-}$$

and $$A(\nu) = A(-\nu)$$

which implies $b_- = 0$, $B_-(\nu) = 0$. Since $B_-(\nu)$ is zero, $B_+(\nu)$ is replaced by $B(\nu)$ to achieve simplicity in notation. Hence eqn. (3.17) reduces to

$$B(\nu) = -\frac{c}{2}\ \bar{f}\ (c,\nu) \int_0^1 X(-\nu')\ e^{-2b/\nu'}$$

$$\times\ \nu'\left(\frac{1}{\nu+\nu'} + h_+(c,\nu,b)\right) B(\nu')\ d\nu' \qquad (3.18)$$

where,

$$\bar{f}(c,\nu) = (c-1)\ g(c,\nu)\ X(-\nu)\ (\nu^2 + k_0^2)$$

When $c > 1$, ν_0 is imaginary and the kernel of eqn. (3.18) can be further simplified by $\nu_0 = ik_0$, where k_0 is a real quantity.

Define,

$$h_+(c,\ \nu,\ b) = \frac{\dfrac{e^{2z_0/\nu_0}}{\nu_0 - \nu} - \dfrac{e^{-2b/\nu_0}}{\nu_0 + \nu}}{e^{2z_0/\nu_0} + e^{-2b/\nu_0}}$$

$$= \frac{\dfrac{e^{2z_0/ ik_0}}{ik_0 - \nu} - \dfrac{e^{-2b/ik_0}}{ik_0 + \nu}}{e^{2z_0/ik_0} + e^{-2b/ik_0}}$$

Separating $h_+(c,\ \nu,\ b)$ in real and imaginary parts, we get

Real part of $h_+\ (c,\ \nu,\ b)$

$$= - \frac{\{\nu\,(1 + \cos \frac{2z_0+2b}{k_0}) + k_0 \sin \frac{2z_0+2b}{k_0}\}}{(\nu^2 + k_0^2)\,\{1 + \cos (\frac{2z_0+2b_0}{k_0})\}}$$

$$= - \frac{1}{(\nu^2+k_0^2)} \{\ \nu + k_0 \tan \frac{b + z_0}{k_0}\}$$

Imaginary part of $h_+(c,\ \nu\ ,\ b) = 0$

Therefore,

$$h_+(c,\ \nu\ ,\ b) = - \frac{1}{\nu^2 + k_0^2} \{\nu + k_0 \tan \frac{b + z_0}{k_0}\}$$

With this simplification, eqn. (3.18) takes the form

$$B(\nu) = \frac{c}{2}\, \bar{f}\ (c,\nu) \int_0^1 X(-\nu')\ e^{-2b/\nu'}$$
$$\times\ \nu' \left[\frac{\nu + k_0 \tan \frac{b+z_0}{k_0}}{\nu^2 + k_0^2} - \frac{1}{\nu+\nu'} \right] B(\nu')\ d\nu' \qquad (3.19)$$

Eqns. (3.17) and (3.19) are the final form of Fredholm eqns. we study in the next section.

3.2 The Inverse Eigenvalue Problem:

The eqn. (3.17) is rewritten in the general form of eigenvalue equation as,

$$\lambda B_{\pm}(\nu) = F_{\pm}(c, \nu, b) - \int_0^1 K_{\pm}(\nu, \nu', b)\, B_{\pm}(\nu')\, d\nu' \qquad (3.20)$$

with,

$$K_{\pm}(\nu, \nu', b) = \pm \frac{c}{2} f(c, \nu)\, X(-\nu')\, e^{-2b/\nu'}$$

$$\times\ \nu' \left(\frac{1}{\nu+\nu'} + h_{\pm}(c, \nu, b)\right) \qquad (3.21)$$

and the inhomogeneous term $F_{\pm}(c, \nu, b)$ is

$$F_{\pm}(c, \nu, b) = f(c, \nu) \left[\frac{2}{c\nu} \gamma(\mu_0)\, \phi_{\nu}(\mu_0) + \gamma(\mu_0)\, h_{\pm}(c, \nu, b)\right] \qquad (3.22)$$

For critical problem (eqn. 3.19), the term $F_{\pm}(c, \nu, b)$ is absent and hence the eigenvalue problem is posed as a homogeneous Fredholm equation,

$$\lambda B(\nu) = \int_0^1 K(\nu, \nu', b)\, B(\nu')\, d\nu' \qquad (3.23)$$

with,

$$K(\nu, \nu', b) = \frac{c}{2} \bar{f}(c, \nu)\, X(-\nu')\, e^{-2b/\nu'}$$

$$\times\ \nu' \left[\frac{\nu + k_0 \tan \frac{b+z_0}{k_0}}{\nu^2 + k_0^2} - \frac{1}{\nu+\nu'}\right] \qquad (3.24)$$

The integral operator generated by the kernel $K(\nu, \nu', b)$ in eqn.(3.23) defines a family of operators $\mathbb{K}(b)$ for different values of the eigenvalue parameter b. Thus the eigenvalue $\lambda(b)$ will be dependent on b analytically i.e. as the parameter b changes, the operator $\mathbb{K}(b)$ and its associated eigenvalue and eigenfunction change correspondingly. In the analysis of the eigenvalue equation, it is determined how the eigenvalue $\lambda(b)$ and eigenfunction $B(\nu)$ change with the operator $\mathbb{K}(b)$ i.e. with changes in the parameter b. For a fixed value of the parameter b, the analysis reduces to that of usual Fredholm equation and thus the solution of the eigenvalue problem is straightforward. But, as we have seen, the problem arising in the present study is the inverse of the eigenvalue problem. In such a problem, the eigenvalue λ is specified and the parameter b (i.e. the operator) which produces this eigenvalue has to be determined. Analysis of this kind of problem, unlike the eigenvalue problem, is indeed not simple and straightforward.

3.3 The Critical Problem:

In the present analysis, the critical slab problem is defined by putting $\lambda(b) = 1$ in equation (3.23) i.e. eigenvalue is equal to 1. The parameter b corresponding to $\lambda(b) = 1$ is the critical half-thickness and is the desired quantity of interest. The crux of the present analysis consists in establishing the existence of such a b and seeks to determine this parameter. By putting $\lambda = 1$ in eqn. (3.23), the corresponding eqn. for the critical problem is obtained as,

$$B(\nu) = \int_0^1 K(\nu, \nu', b) \; B(\nu') \, d\nu' \tag{3.25}$$

where $K(\nu, \nu', b)$ is given by equation (3.24).

To proceed with the analysis of eqn.(3.25), we need the following theorem due to Gohberg [48].

Gohberg Theorem:

Let $\mathbb{K}(b)$ be an analytic operator valued function in an open connected set G, whose values are compact operators for $b \varepsilon G$ on the Banach space X. Then for any $\mu \neq 0$, one of the two possibilities must hold (a) for every $b \varepsilon G$, μ is an eigenvalue of $\mathbb{K}(b)$ or, (b) except for a discrete set of values $b_k \varepsilon G$, the operator $\mu \mathbb{I} - \mathbb{K}(b)$ has a bounded every where defined inverse, while $(\mu \mathbb{I} - \mathbb{K}(b))^{-1}$ has a pole at each of the points b_k. We assume that the family of operators $\mathbb{K}(b)$ generated by the kernel $K(\nu, \nu', b)$ acts on an Hilbert space $\mathbb{L}_2(0, 1)$ of continuous positive functions. The spectrum of the operator $\mathbb{K}$ will, in general, consists of a continuous and residual part in addition to the isolated point spectrum which need not be finite. However, the compactness of the operator $\mathbb{K}(b)$ eliminates the continuous and residual spectra and ensures point spectrum only. The integral operator $\mathbb{K}(\nu, \nu', b)$ acting in $\mathbb{L}_2(0, 1)$ will be compact if the corresponding kernel $K(\nu, \nu', b)$ is an $\mathbb{L}_2$ kernel i.e. if

$$\int_0^1 \int_0^1 |K(\nu, \nu', b)|^2 \, d\nu \, d\nu' < \infty \qquad (3.26)$$

Since $\nu, \nu' \varepsilon (0, 1)$, it is trivial that eqn. (3.26) will be satisfied if the kernel $K(\nu, \nu', b)$ has no singularity. This is true in each of the segments,

$$0 \leq \frac{b + z_o}{k_o} < \frac{\pi}{2}$$

and,

$$\frac{n\pi}{2} < \frac{b+z_o}{k_o} < (n+2)\frac{\pi}{2} \qquad n = 1,3,5,\ldots$$

In the derivation of eqn. (3.23), the slab thickness b has been assumed to have positive real values. Mathematically also, negative values of b are not allowed. This is because the factor $e^{-2b/\nu'}$ in the kernel $K(\nu, \nu', b)$ in the neighbourhood of $\nu' = 0$, for negative b makes the kernel unbounded and thus eqn. (3.26) is no longer satisfied. Summarizing the results, we find that $\mathbb{K}(b)$ is an analytic operator valued function in the open-connected set G either in the range $0 \leq \frac{b+z_o}{k_o} < \pi/2$ or $\frac{n\pi}{2} < \frac{b+z_o}{k_o} < (n+2)\frac{\pi}{2}$ $n = 1,3,5,\ldots$ whose values are compact operators for $b \varepsilon G$ on $\mathbb{L}_2(0, 1)$. It can now be concluded that the conditions for applicability of Gohberg theorem are satisfied in the present case. The theorem is to be applied in the range of $0 \leq \frac{b+z_0}{K_0} < \frac{\pi}{2}$ for our purpose. According to the theorem, one of the two possibilities must hold a) for every $b \in G$, 1 is the eigenvalue of the operator eqn. (3.25) $B = \mathbb{K}(b)\, B$ or b) except for a discrete set of $b_k \in G$, the operator $\mathbb{I} - \mathbb{K}(b)$ has a bounded every-where defined inverse, while $(\mathbb{I} - \mathbb{K}(b))^{-1}$ has a pole at each of the points b_k. The operator $\mathbb{K}(b)$ is obviously a bounded operator and hence from eqn. (3.25),

$$\| B \| = \| \mathbb{K} B \| \leq \| \mathbb{K} \| \; \| B \| \tag{3.27}$$

For a nontrivial B to exist, it follows from eqn.(3.27) that

$$\| \mathbb{K} \| \geq 1$$

$$\text{i.e.} \quad \int_0^1 \int_0^1 | K(\nu, \nu', b) |^2 \, d\nu \, d\nu' \geq 1 \tag{3.28}$$

is the necessary condition for nontrivial solution of B. However, for b = 0, it is seen from numerical calculation that $K(\nu, \nu', b)$ is always less than 1. Table 3.1 shows the values of $K(\nu, \nu', b)$ for different values of c, and b = 0. Hence, for b = 0 $\| \mathbb{K} \|$ is always less than 1 and it is concluded, 1 cannot be an eigenvalue of eqn. (3.25) for b = 0. The first possibility (a) thus cannot be applicable and consequently possibility (b) must hold. This proves the existence of atleast one b_k (i.e. the critical thickness)

Table 3.1(a): $K(\nu, \nu', b)$ as a function of ν, ν' for $c = 1.1$, $b = 0$.

ν \ ν'	0.0	0.2	0.4	0.6	0.8	1.0
0.0	-0.2689	-0.3697	-0.2894	-0.2387	-0.2005	-0.1674
0.2	0.0000	-0.1211	-0.1241	-0.1128	-0.0988	-0.0837
0.4	0.0000	-0.0562	-0.0634	-0.0600	-0.0531	-0.0447
0.6	0.0000	-0.0234	-0.0333	-0.0318	-0.0279	-0.0227
0.8	0.0000	-0.0133	-0.0158	-0.0149	-0.0127	-0.0097
1.0	0.0000	-0.0000	-0.0000	-0.0000	0.0000	0.0000

Table 3.1(b): $K(\nu, \nu', b)$ as a function of ν, ν' for $c = 1.3$ and $b = 0$.

ν \ ν'	0.0	0.2	0.4	0.6	0.8	1.0
0.0	−0.3150	−0.3830	−0.2580	−0.1797	−0.1195	−0.0740
0.2	0.0000	−0.1000	−0.0782	−0.0478	−0.0185	0.0068
0.4	0.0000	−0.0326	−0.0213	−0.0034	0.0147	0.0313
0.6	0.0000	−0.0099	−0.0017	0.0100	0.0218	0.0329
0.8	0.0000	−0.0018	0.0035	0.0104	0.0172	0.0237
1.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3.1(c): $K(\nu, \nu', b)$ as a function of ν, ν' for $c = 1.6$, $b = 0$.

$\nu \setminus \nu'$	0.00	0.2	0.4	0.6	0.8	1.0
0.0	-0.3773	-0.3650	-0.1702	-0.0436	0.0504	0.1233
0.2	0.0000	-0.0483	0.0147	0.0775	0.1297	0.1744
0.4	0.0000	0.0054	0.0427	0.0811	0.1135	0.1423
0.6	0.0000	0.0122	0.0349	0.0582	0.0779	0.0958
0.8	0.0000	0.0087	0.0208	0.0331	0.0437	0.0534
1.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3.1(d): K(ν, ν', b) as a function of ν, ν',
for c = 2 and b = 0.

ν \ ν'	0.0	0.2	0.4	0.6	0.8	1.0
0.0	-0.4700	-0.3016	0.0129	0.2179	0.3680	0.4822
0.2	0.0000	0.0402	0.1668	0.2746	0.3623	0.4321
0.4	0.0000	0.0513	0.1181	0.1769	0.2264	0.2668
0.6	0.0000	0.0317	0.0664	0.0976	0.1245	0.1468
0.8	0.0000	0.0163	0.0331	0.0485	0.0620	0.0735
1.0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

in the range of $b \varepsilon (0, \frac{\pi}{2} k_o - z_o)$ for which 1 is the eigenvalue of eqn.(3.25) and thus the criticality problem has a non-trivial solution. The outcome of the results of Gohberg theorem leads to an important conclusion. It is to be noted that $\frac{\pi}{2} k_o - z_o$ is the end-point critical half-thickness $b_{end-point}$ [5]. By the present analysis it is proved that the exact critical half-thickness b_c is atleast less than $b_{end-point}$. (This is actually true as evident from exact critical thickness calculation by S_N-method.)

3.4 Numerical Calculation of Critical Thickness by Spectral Radius Method:

As has been mentioned in Chapter I, the present approach of calculation of critical thickness is by no means a competitor to the fast converging Neumann series solution of Mitsis [15], but this method may, however, be addressed to such situations where numerical calculation of the inverse parameter is not otherwise possible or in cases where the Neumann Series solution converges slowly. We start with the concept of spectral radius for a linear operator $\mathbb{K}$. It is proved in the theory of linear operators that the limit

$$r = \lim_{n \to \infty} \sqrt[n]{\| \mathbb{K}^n \|}$$

exists and is finite. The number r is called the spectral radius of the bounded linear operator $\mathbb{K}$.

The spectral radius r is characterized by the fact that the inequality

$$|\lambda| > r$$

implies that the operator $(\mathbb{K} - \lambda \mathbb{I})^{-1}$ exists and is bounded. In particular, if $\mathbb{K}$ is compact, then $r = |\lambda_o|$, where λ_o is an eigenvalue of $\mathbb{K}$ with maximum absolute value. In this analysis, the operator $\mathbb{K}$ as defined by eqn. (3.25) is a compact operator and hence the spectral radius r(b) is equal to the eigenvalue 1 i.e.,

$$r(b) = 1$$

Further if the operator $\mathbb{K}$ is a positive operator, fairly accurate estimates of bounds on spectral radius can be obtained. The operator $\mathbb{K}$ is positive if it leaves a cone $\mathbb{C}$ invariant. A set $\mathbb{C} \subset \mathbb{E}$ where $\mathbb{E}$ is a real Banach space is called a cone if the following conditions are satisfied a) if $u, v \varepsilon \mathbb{C}$, then $\alpha u + \beta v \varepsilon \mathbb{C}$ for all $\alpha, \beta \geq 0$ b) if $u \varepsilon \mathbb{C}$ and $-u \varepsilon \mathbb{C}$ then $u = 0$. The set of non-negative functions in a function space and the set of vectors with non-negative components are examples of cones. The criterion for positivity of an operator $\mathbb{K}$ then can be expressed by saying that if $x \varepsilon \mathbb{C}$ then $\mathbb{K} x \varepsilon \mathbb{C}$. In case of an integral operator acting on the cone of non-negative continuous functions (as in our case), the positivity of the operator is met if the kernel is positive i.e.,

$$K(\nu, \nu') > 0$$

for all ν, ν' in their domain of definition Ω on the set of positive real numbers. For such an integral operator, it can be shown [49]

$$r \leq \max_{\nu\in\Omega} \int_\Omega K(\nu, \nu')\, d\nu'$$

and,

$$r \geq \min_{\nu\in\Omega} \int_\Omega K(\nu, \nu')\, d\nu' \qquad (3.29)$$

The coarse estimates of spectral radius can be further modified as,

$$r \leq \max_{\nu\in\Omega} \frac{\int_\Omega\int_\Omega K(\nu, \nu')\, K(\nu', \tau)\, d\nu'\, d\tau}{\int_\Omega K(\nu, \nu')\, d\nu'}$$

and,

$$r \geq \min_{\nu\in\Omega} \frac{\int_\Omega\int_\Omega K(\nu, \nu')\, K(\nu', \tau)\, d\nu'\, d\tau}{\int_\Omega K(\nu, \nu')\, d\nu'} \qquad (3.30)$$

From eqns. (3.29) and (3.30) the actual spectral radius can be approximated as the average

$$r \approx \frac{1}{2} \left[\max_{\nu\in\Omega} \int_\Omega K(\nu, \nu')\, d\nu' + \min_{\nu\in\Omega} \int_\Omega K(\nu,\nu')\, d\nu' \right] \qquad (3.31a)$$

and,

$$r \approx \frac{1}{2} \left[\max_{\nu\in\Omega} \frac{\int_\Omega\int_\Omega K(\nu, \nu')\, K(\nu', \tau)\, d\nu'\, d\tau}{\int_\Omega K(\nu, \nu')\, d\nu'} + \min_{\nu\in\Omega} \frac{\int_\Omega\int_\Omega K(\nu, \nu') K(\nu', \tau)\, d\nu'\, d\tau}{\int_\Omega K(\nu, \nu')\, d\nu'} \right] \qquad (3.31b)$$

The crude approximation of spectral radius given by eqn. (3.31a), however, gives a fairly accurate estimate of the largest eigenvalue of a Fredholm operator as the following examples show. The eigenvalue obtained by eqn. (3.31a) is denoted as $\bar{\lambda}$.

a) $K(\nu, \nu') = e^{\nu+\nu'}; \nu, \nu' \varepsilon (0, 1)$

$$\bar{\lambda} = \frac{1}{2}(e^2-1) = \lambda \quad \text{(exact value)}$$

b) $K(\nu, \nu') = \nu + \nu'; \nu, \nu' \varepsilon (0, 1)$

$$\bar{\lambda} = 1.00, \quad \lambda = 1.077$$

c) $K(\nu, \nu') = \frac{1}{2}\nu'(2-\nu); \quad \nu, \nu' \varepsilon (0, 1)$

$$\lambda = 0.375 \quad \lambda = 0.333$$

The estimates of spectral radius as given by eqn. (3.31a) will now be applied for the criticality eqn. (3.25) to obtain an approximate numerical estimate of critical thickness.

The eqn. (3.25) is rewritten here for the purpose of analysis,

$$B(\nu) = \int_0^1 K(\nu, \nu', b) \; B(\nu') \, d\nu' \qquad (3.25)$$

with,

$$K(\nu, \nu', b) = \frac{c}{2} \; \bar{f}(c, \nu) \; X(-\nu') \, e^{-2b/\nu'}$$

$$\times \; \nu' \left[\frac{\nu + k_0 \tan \frac{b+z_0}{k_0}}{\nu^2 + k_0^2} - \frac{1}{\nu+\nu'} \right] \qquad (3.24)$$

Unfortunately, the kernel given by eqn. (3.24) is not positive for all ν, $\nu' \varepsilon (0, 1)$. The positivity of the kernel will be met if

$$\frac{\nu + k_o \tan \frac{b+z_o}{k_o}}{\nu^2 + k_o^2} \geq \frac{1}{\nu+\nu'}$$

i.e. if $$\nu' \geq \frac{\nu^2 + k_o^2}{\nu + k_o \tan \frac{b+z_o}{k_o}} - \nu$$

$$= \frac{k_o^2 - \nu k_o \tan \frac{b+z_o}{k_o}}{\nu + k_o \tan \frac{b+z_o}{k_o}}$$

Since the right hand side has a maximum value at $\nu = 0$ for $\nu \varepsilon (0, 1)$ the positivity criterion reduces to

$$\nu' \geq \frac{k_o}{\tan \left(\frac{b+z_o}{k_o}\right)}$$

Thus the kernel $K(\nu, \nu', b)$ (and hence the operator $\mathbb{K}$) is positive for all b in the range of $\nu \varepsilon (0, 1)$ and ν' belonging to the sub-set $(\nu_L(b), 1)$ of $(0,1)$ where

$$\nu_L(b) = \frac{k_o}{\tan \left(\frac{b+z_o}{k_o}\right)} \qquad (3.32)$$

However, for a Fredholm operator, the domain of definition of ν, ν' should be the same. Hence both ν, ν' are allowed only in the interval $(\nu_L(b), 1)$, which is obviously a conservative estimate. (In appendix, it has been shown that further lowering of $\nu_L(b)$ is, indeed, possible.) From eqn. (3.32), it follows,

$$b = k_o \tan^{-1} \left(\frac{k_o}{\nu_L}\right) - \ddot{z}_o \qquad (3.33)$$

By putting maximum possible value of $\nu_L = 1$, eqn. (3.33) gives a lower bound for critical half-thickness as

$$b_L = k_o \tan^{-1}(k_o) - \ddot{z}_o \qquad (3.34)$$

whereas the upper bound has already been derived from Gohberg theorem as,

$$b_U = \frac{\pi}{2} k_o - z_o$$

At the end-point critical half-thickness, it is observed from eqn. (3.32) that $\nu_L(b_{\text{end-point}}) = 0$. Since the end-point result is fairly accurate, it can be reasonably assumed that $\nu_L(b)$ will not be substantially different from zero when b is the exact critical half-thickness. This fact will be reflected by numerical calculation to follow in the next section.

In order to ensure positivity of the operator $\mathbb{K}$, we had to slightly deviate from the original problem, i.e., we do not solve the exact problem as posed by eqn.(3.25) but the following approximate one

$$B(\nu) = \mathbb{K}_{ap}(b)\, B(\nu)$$

where,

$$\mathbb{K}_{ap}\, B(\nu) = \int_{\nu_L}^{1} K(\nu, \nu', b)\, B(\nu')\, d\nu'$$

From eqn. (3.31a), it follows

$$r(b) = \frac{r_{max}(b) + r_{min}(b)}{2} \tag{3.35}$$

where,

$$r_{max}(b) = \max_{\nu \epsilon (0,1)} \int_{\nu_L(b)}^{1} K(\nu, \nu', b)\, d\nu'$$

and

$$r_{min}(b) = \min_{\nu \epsilon (0,1)} \int_{\nu_L(b)}^{1} K(\nu, \nu', b)\, d\nu'$$

The critical half-thickness is given by the eqn.

$$r(b) = 1 \tag{3.36}$$

The integral $\int_{\nu_L(b)}^{1} K(\nu, \nu', b)\, d\nu'$ can be evaluated as

$$\begin{aligned} I(\nu, b) &= \int_{\nu_L(b)}^{1} K(\nu, \nu', b)\, d\nu' \\ &= \frac{c}{2}\, \ddot{f}\,(c, \nu)\, \frac{\nu + k_o \tan \frac{b+z_o}{k_o}}{\nu^2 + k_o^2}\, I_1(b) \\ &\quad - \frac{c}{2}\, \ddot{f}\,(c, \nu)\, I_2(\nu, b) \end{aligned} \tag{3.37}$$

where,

$$I_1(b) = \int_{\nu_L(b)}^{1} \nu' X(-\nu') e^{-2b/\nu'} d\nu'$$

and, $$I_2(\nu, b) = \int_{\nu_L(b)}^{1} \frac{\nu'}{\nu+\nu'} X(-\nu') e^{-2b/\nu'} d\nu'$$

The integrals $I_1(b)$ and $I_2(\nu, b)$ can be obtained numerically with $X(-\nu')$ given by eqn. (3.16). However, to get around the time-consuming numerical integration, $I_1(b)$ and $I_2(\nu, b)$ are approximated in the present analysis as

$$I_1(b) \approx X(-1) e^{-2b} \left(\frac{1-\nu_L^2(b)}{2}\right)$$

$$I_2(\nu, b) \approx X(-1) e^{-2b} \left[1 - \nu_L(b) - \nu \ln \frac{\nu+1}{\nu+\nu_L(b)}\right]$$

Thus, $I(\nu, b)$ is approximated as

$$I(\nu, b) \approx \frac{c}{2} e^{-2b} X(-1) \bar{f}(c, \nu)\left\{ \frac{\nu + k_o \tan \frac{b+z_o}{k_o}}{2(\nu^2 + k_o^2)} \right.$$

$$\left. \times (1 - \nu_L^2(b)) - \left[(1-\nu_L(b) - \nu \ln \frac{\nu+1}{\nu+\nu_L(b)}\right]\right\}$$

$$\nu \,\varepsilon\, (\nu_L(b), 1) \quad (3.38)$$

The constants k_o, z_o, $g(c, \nu)$ needed for evaluation of $I(\nu, b)$ in eqn.(3.38) are taken from Case, de Hoffmann and Placzeck [23].

Eqn. (3.35) is infact a transcendental equation in b and the bisection method is employed for evaluation of b. A value of $b = b_1$ is first chosen in the range of $b_L < b < b_U$ and $I(\nu, b)$ is calculated from eqn. (3.38) for 21 points of ν in the interval $(\nu_L, 1)$. The maximum of these values give r_{max} while the minimum corresponds to r_{min}. The spectral radius is then calculated from eqn.(3.35). If $r(b_1)$ is equal to 1 within a specified error limit (in the present calculation this limit is taken as $\varepsilon = |r(b)-1| = 10^{-5}$), then this choice of $b = b_1$ is the desired critical half-thickness b_c. If the convergence criterion is not met i.e. $r(b_1) \neq 1$, then another value of $b = b_2$ is chosen such that $r(b_2) - 1$ is of opposite sign to $r(b_1) - 1$. The bisection method is then continued to achieve the desired convergence in spectral radius. The corresponding value of b is the critical half-thickness b_c. Numerical results of this calculation alongwith P_1 and P_3 values are shown in Table 3.2. ν_L values at $b = b_c$ for different c are also given in the table. It is observed from numerical values of ν_L that the approximate problem does not differ significantly from the original one for the range of practical values of c (≤ 1.6). Considering the crudity of bounds of spectral radius used here, the results obtained by the present method can be considered to be fairly accurate. The error in critical thickness increases with increasing value of c. This fact is

Table 3.2: Critical half-thickness b_c in units of mean free path.

c	Present (% error)	P_1 (% error)	P_3 (% error)	Exact	(ν_L)
1.02	5.6655 (0.000)	5.7519 (-1.525)	5.6711 (-0.099)	5.6655	0.0000
1.05	3.3002 (0.000)	3.4034 (-3.438)	3.3066 (-0.193)	3.3002	0.0000
1.1	2.1125 (0.043)	2.2287 (-5.454)	2.1213 (-0.376)	2.1134	0.0008
1.2	1.2855 (0.295)	1.4125 (-9.555)	1.3020 (-0.985)	1.2893	0.0043
1.4	0.7231 (1.833)	0.8581 (-15.54)	0.7577 (-2.860)	0.7366	0.0137
1.6	0.4927 (3.769)	0.6269 (-22.44)	0.3394 (-5.151)	0.5120	0.0225
1.8	0.3634 (6.509)	0.4965 (-27.73)	0.4182 (-7.592)	0.3887	0.0298
2.0	0.2805 (9.749)	0.4121 (-32.59)	0.3420 (-10.05)	0.3108	0.0359

not surprising. With increasing value of c, ν_L deviates more from zero and naturally the approximate problem is not that close to the original one as compared to lower values of c. However, the critical thickness significantly improves if integrations in eqn. (3.37) are performed numerically instead of using eqn. (3.38). In this case, the error for c = 2.0 reduces to 7.876 percent from 9.749 per cent. Numerical integration is, however, not recommended because of much greater computational time.

3.5 The Slab Albedo Problem:

For the analysis of the slab albedo problem we consider the eqn. (3.20) with $\lambda = 1$

$$B_{\pm}(\nu) = F_{\pm}(c, \nu, b) - \int_0^1 K_{\pm}(\nu, \nu', b)\, B_{\pm}(\nu')\, d\nu' \quad (3.39)$$

The kernel $K_{\pm}(\nu, \nu', b)$ is given by eqn. (3.21). For $B_+(\nu)$, $K_+(\nu, \nu', b)$ is always positive for $\nu, \nu' \in (0, 1)$ and for all b. Thus the homogeneous eqn.

$$B_+(\nu) = -\int_0^1 K_+(\nu, \nu', b)\, B_+(\nu')\, d\nu'$$

cannot have a nontrivial solution in the cone of positive functions as the eigenvalue in this case is -1. Since $B_+(\nu)$ is a linear combination of $A(\nu)$ and $A(-\nu)$ as seen from eqn. (3.10), $A(\nu)$ and $A(-\nu)$ are also non-existent and thus $B_-(\nu)$ of the homogeneous equation also does not exist. By Fredholm alternative theorem [50], it can then be concluded that $B_{\pm}(\nu)$ of inhomogeneous eqn. (3.39) have unique non-trivial solutions. Looking this from another angle, this can also be shown as follows. $B_-(\nu)$ satisfies the following equation,

$$B_-(\nu) = F_-(c,\nu,b) + \int_0^1 K_-(\nu,\nu',b)\, B_-(\nu')\, d\nu' \qquad (3.40)$$

where the kernel $K_-(\nu,\nu',b)$ of eqn. (3.21) is redefined as

$$K_-(\nu,\nu',b) = \frac{c}{2} f(c,\nu)\, X(-\nu')\, e^{-2b/\nu'}$$

$$\times\ \nu' \left(\frac{1}{\nu+\nu'} + h_-(c,\nu,b)\right)$$

We consider the governing eqn. for $B_-(\nu)$ only as we find $K_-(\nu,\nu',b) > K_+(\nu,\nu',b)$ and any inference drawn on $B_-(\nu)$ in this analysis will hold for $B_+(\nu)$ also. To show that $B_-(\nu)$ has a unique non-trivial solution, we proceed as follows:

An equation of the form

$$\lambda x = \mathbb{K}\, x + f \qquad (3.41)$$

has a unique solution

$$x = (\lambda\, \mathbb{I} - \mathbb{K})^{-1} f \qquad (3.42)$$

if $\quad |\lambda| >$ spectral radius $\qquad$ (3.43)

From eqn. (3.29), the upper bound for spectral radius r can be estimated in our case as,

$$r \leq \max_{\nu\epsilon(0,1)} \int_0^1 K_{-}(\nu, \nu', b) \; d\nu'$$

$$= \max_{\nu\epsilon(0,1)} \frac{c}{2} f(c,\nu) \int_0^1 e^{-2b/\nu'} X(-\nu')$$

$$\times \nu \left(\frac{1}{\nu+\nu'} + h_{-}(c,\nu, b)\right) d\nu'$$

$$\leq \max_{\nu\epsilon(0,1)} \frac{c}{2} f(c,\nu) \; X(-1) \; e^{-2b}$$

$$\times \left[\int_0^1 \frac{\nu'}{\nu+\nu'} d\nu' + h_{-}(c,\nu, b) \int_0^1 \nu' d\nu'\right]$$

$$\leq \max_{\nu\epsilon(0,1)} \left\{ \frac{c}{2} f(c,\nu) \; X(-1) \; e^{-2b} \; h_{-}(c,\nu, b) \; \frac{1}{2}\right.$$

$$\left. + \frac{c}{2} f(c,\nu) \; X(-1) \; e^{-2b} \left(1 - \nu \ln \frac{1+\nu}{\nu}\right)\right\}$$

$$= \max_{\nu\epsilon(0,1)} I_3(\nu, b)$$

The right hand side $I_3(\nu, b)$ is calculated numerically for different values of $c < 1$ and for different values of b for 21 points of ν in (0, 1) starting from $\nu = 0$, at an interval of .05. The results are shown in Table 3.3. Maximum value is always found to be less than 1 and hence the spectral radius is less than 1. From eqn. (3.40), it follows $|\lambda| = 1$ and so, condition (3.43) is satisfied. Hence, eqn.(3.40) has a unique solution for $B_{-}(\nu)$. In other words, the slab albedo problem has a unique solution for all $c < 1$ and for all b. The restriction relating b

Table 3.3(a): $I_3(\nu, b)$ as a function of ν for $b = 0.5$ and $c = 0.9, 0.6, 0.2$.

ν	c		
	0.9	0.6	0.2
0.00	0.0848	0.0649	0.0256
0.05	0.0676	0.0536	0.0219
0.10	0.0578	0.0472	0.0197
0.15	0.0507	0.0425	0.0181
0.20	0.0452	0.0389	0.0168
0.25	0.0407	0.0360	0.0158
0.30	0.0369	0.0337	0.0149
0.35	0.0337	0.0317	0.0142
0.40	0.0309	0.0301	0.0136
0.45	0.0284	0.0288	0.0131
0.50	0.0265	0.0276	0.0127
0.55	0.0241	0.0267	0.0124
0.60	0.0222	0.0259	0.0121
0.65	0.0204	0.0253	0.0120
0.70	0.0187	0.0248	0.0119
0.75	0.0169	0.0244	0.0120
0.80	0.0151	0.0241	0.0122
0.85	0.0132	0.0238	0.0127
0.90	0.0110	0.0232	0.0136
0.95	0.0082	0.0212	0.0159
1.00	0.0000	0.0000	0.0000

Table 3.3(b): $I_3(\nu, b)$ as a function of ν for $b = 1.0$ and $c = 0.9, 0.6, 0.2$.

ν	c		
	0.9	0.6	0.2
0.00	0.0293	0.0234	0.0094
0.05	0.0232	0.0193	0.0081
0.10	0.0197	0.0170	0.0073
0.15	0.0172	0.0153	0.0067
0.20	0.0153	0.0140	0.0062
0.25	0.0137	0.0130	0.0058
0.30	0.0124	0.0121	0.0055
0.35	0.0113	0.0114	0.0052
0.40	0.0103	0.0108	0.0050
0.45	0.0095	0.0103	0.0048
0.50	0.0088	0.0099	0.0047
0.55	0.0080	0.0096	0.0046
0.60	0.0074	0.0093	0.0045
0.65	0.0068	0.0091	0.0044
0.70	0.0062	0.0089	0.0044
0.75	0.0056	0.0087	0.0044
0.80	0.0050	0.0086	0.0045
0.85	0.0043	0.0085	0.0047
0.90	0.0036	0.0083	0.0050
0.95	0.0027	0.0076	0.0058
1.00	0.0000	0.0000	0.0000

and c as obtained by McCormick and Mendelson [17] is only necessary for the Neumann Series solution to converge and not for a solution to exist.

CHAPTER IV

MODIFICATION AND SUGGESTIONS

Introduction:

In this chapter, an attempt has been made to rectify some of the shortcomings as appeared in the development of Chapter II. It is concluded in Chapter II that the TP_N-formulalism based on source-free Milne problem does not necessarily improve the leakage for the constant source Milne problem for strong absorption cases. The reason for this is attributed to the fact that the extrapolation distance for constant source problem is widely different from that of source-free Milne problem for low values of c. This necessitates a separate formulation of TP_N approximation based on constant source Milne problem in those cases where the source-free Milne problem cannot be considered as the standard reference problem. Here, an expression for the extrapolation distance for constant source problem has been derived by application of Case's theory. TP_1 formulation based on constant source problem is then constructed by introducing a parameter ε_1 in the Marshak free-surface condition in a similar manner as in Chapter II. The parameter ε_1 is determined by equating the leakage from the half-space in TP_1 approximation to the exact leakage. The formalism can be easily extended for higher order approximations. However, it has not been undertaken in the present work. The purpose of the present work is simply to demonstrate that the source-free Milne problem should not be taken as the only standard reference problem for construction of the TP_N equations. The scheme can be applied for any practical problem which can be approximately represented by a constant source type problem such as computation of thermal worth of a control element in an assembly. In this chapter, the escape probability for a finite slab containing a source has been calculated by the present method and compared with the results of conventional P_1 approximation and exact analysis. It has been demonstrated that the present formulation improves the results whereas the TP_1 approximation based on source-free Milne problem fails for strong absorption cases.

4.1 Analysis:

For the constant source half-space problem, the extrapolation distance is obtained by equating the asymptotic flux to zero as follows [5]

$$\frac{2q_o}{(1-c)} + a_{o+}\, e^{-z_o^{cs}/\nu_o} = 0 \qquad (4.1)$$

where,

$$a_{0+} = \frac{2q_0}{(1-c)\ c\ \nu_0\ X(\nu_0)} \tag{4.2}$$

q_0 is a uniform isotropic source

ν_0 is given by the positive root of

$$\frac{c\nu}{2} \ln \frac{\nu+1}{\nu-1} = 1$$

We already have,

$$X(\nu_0) = -e^{z_0/\nu_0} \sqrt{\frac{1-\nu_0^2\ (1-c)}{2\nu_0^2\ (1-c)\ (\nu_0^2-1)}} \tag{4.3}$$

z_0^{cs} is then obtained from eqns. (4.1), (4.2) and (4.3) as

$$cz_0^{cs} = cz_0 + \frac{c\nu_0}{2} \ln \left\{ \frac{c^2\ [\nu_0^2\ (c-1) + 1]}{2(1-c)\ (\nu_0^2-1)} \right\} \tag{4.4}$$

Table 4.1 compares the values of z_0^{cs} as obtained from eqn. (4.4) with z_0. It is found that for low values of c, z_0^{cs} is widely different from z_0. Thus, TP_1-approximation normalized to exact asymptotic flux of source-free Milne problem (i.e. exact z_0) may lead to significant errors for constant source type problem in case of strong absorption. This calls for a separate formulation for this class of problems. However, unlike TP_1 theory developed in Chapter II, the present formalism is not normalized to exact asymptotic

Table 4.1: Constant-Source Milne problem extrapolation distance z_o^{cs} and source-free Milne problem extrapolation distance z_o.

c	cz_o^{cs}	cz_o
0.0	2.000	1.000
0.1	1.4097	0.8539
0.2	1.1162	0.7851
0.3	0.9439	0.7491
0.4	0.8418	0.7305
0.5	0.7792	0.7205
0.6	0.7401	0.7155
0.7	0.7158	0.7127
0.8	0.7023	0.7113
0.9	0.6977	0.7106
1.0	0.7104	0.7104

flux. The reason for this is the following. The use of exact asymptotic flux in constant source problem yields an infinite linear extrapolation distance for the purely absorption case [51]. It has been found [51] that the use of this linear extrapolation distance when used in asymptotic diffusion theory would yield zero control rod worth. In order to circumvent this unrealistic situation, the present formulation is normalized to exact leakage from an half-space and not to the exact asymptotic flux. It is to be noted that this problem does not arise for source-free Milne problem in which case the extrapolation distance has a finite value as c → 0.

TP_1 flux for the constant source Milne problem is given as,

$$\psi(x, \mu) = \frac{q_o}{(1-c)} + a_{o+} \phi_{o+}(\mu)\, e^{-x/\nu_o} \qquad (4.5)$$

The leakage from the half-space is obtained from the above eqn. as,

$$L = \int_{-1}^{1} \mu\, \psi(0, \mu)\, d\mu = a_{o+}^{(1)}\, g_1(\nu_o) \qquad (4.6)$$

The Marshak free-surface condition is modified by introducing a parameter ε_1 in the following manner,

$$\int_{o}^{1} (\mu+\varepsilon_1)\, \psi(0, \mu)\, d\mu = 0 \qquad (4.7)$$

By use of eqn. (4.5), the expression for ε_1 is obtained from condition (4.7) as

$$\varepsilon_1 = - \frac{\frac{q_o}{2(1-c)} + a_{o+}^{(1)} \frac{c\nu_o}{2} \{\nu_o \ln \frac{\nu_o}{\nu_o - 1} - 1\}}{\frac{q_o}{(1-c)} + a_{o+}^{(1)} \frac{c\nu_o}{2} \ln \frac{\nu_o}{\nu_o - 1}} \tag{4.8}$$

The coefficient $a_{o+}^{(1)}$ is obtained by forcing the TP_1 leakage equal to exact leakage as

$$L^{(T1)} = L_{exact} = - \frac{2q_o}{c} [\nu_o - I(c)] \tag{4.9}$$

By use of eqn.(4.6), $a_{o+}^{(1)}$ is obtained from eqn. (4.9) as

$$a_{o+}^{(1)} = - \frac{2q_o}{cg_1(\nu_o)} [\nu_o - I(c)] \tag{4.10}$$

Substituting $a_{o+}^{(1)}$ from eqn. (4.10) into eqn. (4.8) ε_1 simplifies to

$$\varepsilon_1(c) = - \frac{\{\nu_o - I(c)\} \{\nu_o \ln \frac{\nu_o}{\nu_o - 1} - 1\} - \frac{1}{2}}{\{\nu_o - I(c)\} \ln \frac{\nu_o}{\nu_o - 1} - 1} \tag{4.11}$$

The function I(c) is tabulated by Case, de Hoffmann and Placzeck [23]. The limiting values of $\varepsilon_1(c)$ for pure scattering case is obtained by a limiting procedure to be

$$\varepsilon_1(1) = - \frac{3\, I(1) - 2}{3(2I(1) - 1)} = - 0.1039$$

In order to avoid a lengthy limiting procedure for pure absorption case, $\varepsilon_1(0)$ is simply evaluated by extrapolation. This is found to be equal to -0.0035. Due to extreme insensitiveness of ν_o value with c for high absorptions, it is recommended that $\varepsilon_1(c)$ should be evaluated by simple linear interpolation for values of c between 0 and 0.2. Numerical values of ε_1 for different values of c are given in Table 4.2. For any problem involving free-surface and representing a constant source-type problem, $\varepsilon_1(c)$ as evaluated from eqn.(4.11) is used. The coefficient $a_{o+}^{(1)}$ can then be obtained from Marshak free-surface condition (4.7). The formalism is now applied for computing escape probability P for a finite slab.

4.2 Escape Probability for a Finite Slab:

We consider a homogeneous slab of half-thickness b with a spatially constant source and the rest of the space considered as a purely absorbing medium. The angular density $\psi(x, \mu)$ for TP_1-approximation, with the origin of coordinate at the centre of the slab, is given by,

$$\psi(x, \mu) = \frac{q_o}{(1-c)} + a_{o+}^{(1)} \left\{ \frac{c\nu_o}{2(\nu_o-\mu)} e^{-x/\nu_o} + \frac{c\nu_o}{2(\nu_o+\mu)} e^{x/\nu_o} \right\} \qquad (4.12)$$

Table 4.2: $\varepsilon_1(c)$ as a function of c.

c	$\varepsilon_1(c)$
0.0	-0.0035
0.1	-0.0074
0.2	-0.0113
0.3	-0.0164
0.4	-0.0228
0.5	-0.0292
0.6	-0.0368
0.7	-0.0445
0.8	-0.0544
0.9	-0.0679
1.0	-0.1039

The coefficient $a_{o+}^{(1)}$ is obtained from the condition (4.7) as

$$\int_{o}^{1} (\mu + \varepsilon_1) \ \psi(-b, \mu) \, d\mu = 0$$

By use of eqn. (4.12) for $\psi(-b, \mu)$, we get

$$a_{o+}^{(1)} = - \frac{q_o (1+2\varepsilon_1)}{c\nu_o (1-c) \{ (\nu_o+\varepsilon_1) \, e^{b/\nu_o} \ln \frac{\nu_o}{\nu_o-1} - (\nu_o-\varepsilon_1) e^{-b/\nu_o} \ln \frac{\nu_o+1}{\nu_o} - 2 \sinh(b/\nu_o) \}} \qquad (4.13)$$

In eqn. (4.13), ε_1 is used from eqn. (4.11). The escape probability P is defined by,

$$P = 1 - \frac{(1-c) \int_{-b}^{b} \phi(x) \, dx}{4bq_o} \qquad (4.14)$$

The scalar flux $\phi(x)$ from eqn. (4.12) is

$$\phi(x) = \frac{2q_o}{(1-c)} + 2a_{o+}^{(1)} \cosh(x/\nu_o) \qquad (4.15)$$

By use of eqns. (4.14) and (4.15), P is given by

$$P^{(T1)} = - \frac{a_{o+}^{(1)} \sinh\left(\frac{b}{\nu_o}\right) g_1(\nu_o)}{b \, q_o} \qquad (4.16)$$

Substituting $a_{o+}^{(1)}$ from eqn. (4.13), eqn. (4.16) becomes

$$P^{(T1)} = - \frac{(1 + 2\varepsilon_1) \sinh\left(\frac{b}{\nu_o}\right)}{cb \, \{(\nu_o+\varepsilon_1) \, e^{b/\nu_o} \ln \frac{\nu_o}{\nu_o-1} - (\nu_o-\varepsilon_1) \, e^{-b/\nu_o} \ln \frac{\nu_o+1}{\nu_o} - 2 \sinh(b \ \nu_o) \}} \qquad (4.17)$$

Conventional P_1-approximation result is given by,

$$P^{(1)} = \frac{\nu_0^{(1)} \sinh\left(\frac{b}{\nu_0^{(1)}}\right)}{b\left\{\cosh\left(\frac{b}{\nu_0^{(1)}}\right) + 2\, g_1(\nu_0^{(1)}) \sinh\left(\frac{b}{\nu_0^{(1)}}\right)\right\}}$$

Table 4.3 compares the TP_1 values of escape probability with P_1 and exact values. TP_1 values corresponding to source-free Milne problem are also given for comparison. It is found that the present formulation improves the result significantly over conventional P_1-approximation for all values of b and c where as the TP_1-formulation based on source-free Milne problem fails absolutely for low values of c. The exact results for c = 0.6, 0.4 and 0.2 are taken from curves [52] and hence, they could be given only upto two decimal places. The other exact results are taken from reference [26].

4.3 Suggestions:

It has been observed that TP_N formulation based on source-free Milne problem fails in those cases where the transient is overwhelmingly predominant. This is because of the fact that the transient is still in the framework of P_N approximation and the improvement in the asymptotic portion of the solution is offset by a corresponding worsening of the transient part. The conventional P_N approximation,

Table 4.3: Escape probability from a slab, P, as a function of b and c.

c	b	P_1 (% error)	TP_1 (% error)		Exact
			based on constant source Milne problem	based on source-free Milne problem	
0.9	0.5	0.9024 (4.61)	0.8402 (-2.59)	0.8267 (-4.16)	0.8626
	2.0	0.5866 (7.65)	0.5425 (-0.44)	0.5300 (-2.73)	0.5449
	10.0	0.1400 (7.36)	0.1305 (0.07)	0.1272 (-2.45)	0.1304
0.8	0.5	0.8223 (8.34)	0.7237 (-4.65)	0.6839 (-9.89)	0.7590
	2.0	0.4233 (10.72)	0.3803 (-0.52)	0.3547 (-7.22)	0.3823
	10.0	0.0903 (9.85)	0.0823 (0.12)	0.0766 (-6.81)	0.0822
0.6	0.5	0.70	0.56	0.44	0.61
	2.0	0.28	0.24	0.19	0.26
	10.0	0.06	0.05	0.04	0.05
0.5	0.5	0.6499 (16.24)	0.5016 (-10.28)	0.3316 (-40.69)	0.5591
	2.0	0.2408 (14.83)	0.2082 (-0.71)	0.1346 (-35.81)	0.2097
	10.0	0.0486 (14.08)	0.0427 (10.23)	0.0276 (-35.21)	0.0426
0.4	0.5	0.61	0.45	0.23	0.52
	2.0	0.21	0.18	0.09	0.19
	10.0	0.04	0.04	0.02	0.04
0.2	0.5	0.54	0.37	0.09	0.45
	2.0	0.17	0.15	0.04	0.16
	10.0	0.03	0.03	0.01	0.03

being a total theory, may however predict the overall results fairly accurately although the contributions due to asymptotic and transient parts separately are far from the exact results. The improvement of the TP_N-formulation for strong absorption cases, however, may not be possible in the framework of P_N-approximation as has been discussed in Chapter II. A better transient flux representation containing few terms is thus called for.

Spectral radius method of inverse parameter estimation can be applied for some general problems in those cases where the inverse parameter is not otherwise easily available.

No such attempt has, however, been undertaken in the present dissertation.

REFERENCES

1. M.M.R. WILLIAMS: 'The Wiener-Hopf Method - An Alternative to the Singular Eigenfunction Method', in *Advances in Nuclear Science and Technology*, Vol. 7, Academic Press, New York and London, (1973).

2. N. WIENER and E. HOPF, Berlin. Ber. Math.Phys.Kl, 696, (1931).

3. K.M. CASE, Ann. Phys. (New York) **9**, 1, (1960).

4. B. DAVISON, *Neutron Transport Theory*, Oxford Univ. Press, London and New York, (1957).

5. K.M. CASE and P.F. ZWEIFEL, *Linear Transport Theory*, Addison-Wesley Publishing Company, Massachusetts, (1967).

6. G.I. BELL and S. GLASSTONE, *Nuclear Reactor Theory*, Van Nostrand-Reinhold, Princeton, New Jersey, (1970).

7. N.J. McCORMICK and I. KUŜĈER: 'Singular Eigenfunction Expansions in Neutron Transport Theory' in '*Advances in Nuclear Science and Technology*, Vol. 7, Academic Press, New York and London, (1973).

8. J.R. MIKA, Nucl. Sci. Engng. **11**, 415, (1961).

9. M.R. MENDELSON and G.C. SUMMERFIELD, J.Math.Phys. **5**, 668, (1964).

10. S. PAHOR and J.K. SHULTIS, J.Nucl.Energy **23**, 477, (1969).

11. C.E. SIEWERT and Y. ISHIGURO, J. Nucl.Energy **26**, 251, (1972).

12. D.R. METCALF and P.F. ZWEIFEL, Nucl. Sci.Engng. **33**, 307 and 318, (1968).

13. S. PAHOR and J.K. SHULTIS, J.Math. Phys. **10**, 2220, (1969).

14. R.L. BOWDEN and A.G. BULLARD, J.Nucl.Energy **23**, 655, (1969).

15. G.J. MITSIS, Nucl. Sci. Engng. **17**, 55, (1963).

16. N.I. MUSKHELISHVILI, Singular Integral Equations, Noordh off, Groningen, Holland (1953).

17. N.J. McCORMICK and M.R. MENDELSON, Nucl. Sci. Engng. 20, 462, (1964).

18. A. LEONARD and T.W. MULLIKIN, J. Math. Phys. 5, 399,(1964).

19. R.L. BOWDEN, F.J. McCROSSON and E.A. RHODES, J.Math. Phys. 9, 753,(1968).

20. R.C. ERDMANN, J. Nucl. Energy. 23, 53, (1969).

21. R.E. MARSHAK, Phys. Rev. 71, 443, (1947).

22. J.C. MARK, Report MT-97, National Research Council of Canada, Atomic Energy Project, (1945).

23. K.M. CASE, F. de HOFFMANN and G. PLACZEK, Introduction to the Theory of Neutron Diffusion, Los Alamos Scientific Laboratory (1953).

24. G.C. POMRANING and M. CLARK, Nucl. Sci. Engng. 17, 227,(1963).

25. D.S. SELENGUT, Trans. Am. Nucl. Soc. 5, 413,(1962).

26. G.C. POMRANING, Nucl. Sci. Engng. 21, 62, (1965).

27. G.P. CALAME, J. Nucl. Energy 22, 497, (1968).

28. R.J. DOYAS and B.L. KOPONEN, Nucl. Sci. Engng. 41, 226, (1970).

29. W.R. CONKIE, Nucl. Sci. Engng. 6, 267, (1959) and 18, 370, (1964).

30. G.C. POMRANING, Nucl. Sci. Engng. 22, 328, (1965).

31. M. COPIC, Nucl. Sci. Engng. 26, 289 (1966).

32. L.E. BEGHIAN, Nucl. Sci. Engng. 51, 78, (1973).

33. L.K. KIN, High Order Spherical Harmonics Method for Neutron Deep Penetration, Eng. Sc.D. Thesis, Columbia University, (1975).

34. J. LEHNER and G.M. WING, Commun. Pure Appl. Math. 8, 217, (1955) and G.M. WING, 'An Introduction to Transport Theory', Wiley, New York, (1962).

35. S. UKAI, J.Nucl. Energy, 19, 833, (1965).

36. I. VIDAV, J. Math. Anal. Appl. 22, 144, (1968).

37. E.W. LARSEN and P.F. ZWEIFEL, J. Math. Phys. 15, 1987, (1974).

38. I. KUŠČER and I. VIDAV, J. Math. Anal. Appl. 25, 80, (1969).

39. M. G. KREIN and M.A. RUTMAN, Linear Operators Leaving Invariant A Cone in a Banach Space, Uspehi Math. Nauk (N.S.) 3, 3, (1948).

40. W.L. HENDRY, Nucl. Sci. Engng. 30, 306, (1967).

41. E. OBLOW, K. KIN and H. GOLDSTEIN, Nucl. Sci. Engng. 54, 72, (1974).

42. S. CHANDRASEKHAR, Radiative Transfer, Oxford Univ. Press, London, (1950).

43. B.O. PEIRCE, A Short Table of Integrals, Oxford and IBH Publishing Co., (1966).

44. A.M. WEINBERG and E.P. WIGNER, The Physical Theory of Neutron Chain Reactors, The University of Chicago Press, Chicago, (1958).

45. J.C. MARK, Phys. Rev. 72, 558, (1947).

46. P. BENOIST, Nucl. Sci. Engng. 68, 31, (1978).

47. R.L. MURRAY, Nuclear Reactor Physics, Macmillan and Co. Ltd., London, (1959).

48. I.C. GOHBERG and M.G. KREIN, Introduction to the Theory of Linear Nonself-adjoint Operators, Amer. Math. Soc., Providence, R.I., (1969).

49. M.A. KRASNOSEL'SKII, Approximate Solution of Operator Equations, Wolters-Noordhoff Publishing, Groningen (1972).

50. A.E. TAYLOR, Introduction to Functional Analysis, John Wiley and Sons, Inc., New York (1958).

51. G.C. POMRANING, Nucl. Sci. Engng. 16, 239, (1963).

52. D. SCHIFF and S. STEIN, 'Escape Probability and Capture Fractions for Grey Slabs', Report WAPD-149, Westinghouse (1956).

53. H. HURWITZ and P.F. ZWEIFEL, J. Appl. Phys. 26, 923, (1955).

APPENDIX A

CONSTRUCTION OF $g_n(\nu)$ FUNCTIONS FOR ANISOTROPIC SCATTERING

In case of anisotropic scattering the one-speed transport equation is,

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \psi(x, \mu) = \frac{c}{2} \sum_{l=0}^{L} (2l+1) f_l P_l(\mu) \times \int_{-1}^{1} \psi(x, \mu') P_l(\mu') d\mu' \qquad (A1)$$

where the scattering function is approximated by a finite sum of Legendre polynomials and L is the order of anisotropy. In a similar procedure as in isotropic case, we apply the ansatz,

$$\psi(x, \mu) = e^{-x/\nu} \phi_\nu(\mu) \qquad (A2)$$

where,

$$\phi_\nu(\mu) = \sum_{n=0}^{\infty} \frac{2n+1}{2} g_n(\nu) P_n(\mu) \qquad (A3)$$

and, obviously,

$$g_n(\nu) = \int_{-1}^{1} \phi_\nu(\mu) P_n(\mu) d\mu \qquad (A4)$$

By use of Eqn. (A2) in (A1) $\phi_\nu(\mu)$ is obtained as,

$$\phi_\nu(\mu) = \frac{c\nu}{2(\nu-\mu)} \sum_{l=0}^{L} (2l+1)\, f_l\, g_l(\nu)\, P_l(\mu),$$

$$\nu \notin (-1,\ 1) \qquad \text{(A5)}$$

and,

$$\phi_\nu(\mu) = \frac{c\nu}{2}\, P \frac{1}{(\nu-\mu)} \sum_{l=0}^{L} (2l+1)\, f_l\, g_l(\nu)\, P_l(\mu)$$

$$+\ \lambda(\nu)\, \delta(\nu-\mu), \qquad \nu \in (-1,\ 1) \qquad \text{(A6)}$$

Use of eqns. (A3) and (A6) gives $g_n(\nu)$, when $\nu \in (-1,\ 1)$, as

$$g_n(\nu) = \frac{c\nu}{2} \sum_{l=0}^{L} (2l+1)\, f_l\, g_l(\nu)\, P \int_{-1}^{1} \frac{P_l(\mu)\, P_n(\mu)}{(\nu-\mu)}\, d\mu$$

$$+\ \lambda(\nu)\, P_n(\nu) \quad , \qquad \nu \in (-1,\ 1)$$

By utilizing, [53]

$$\int_{-1}^{1} \frac{P_l(\mu)\, P_n(\mu)}{(\nu-\mu)}\, d\mu = 2Q_n(\nu)\, P_l(\nu) \qquad l \leq n \qquad \text{(A7)}$$

We get, when $\nu \in (-1,\ 1)$,

$$g_n(\nu) = c\nu\, P\, Q_n(\nu) \sum_{l=0}^{L} (2L+1)\, f_l\, g_l(\nu)\, P_l(\nu)$$

$$+\ \lambda(\nu)\, P_n(\nu) \qquad n \geq L \qquad \text{(A8)}$$

and,

$$g_n(\nu) = \frac{c\nu}{2} \{ PQ_n(\nu) \sum_{l=0}^{n} (2-\delta_{ln})(2l+1)\, f_l\, g_l(\nu)\, P_l(\nu)$$

$$+ P_n(\nu) \sum_{l=n}^{L} (2-\delta_{ln})\, (2l+1)\, f_l\, g_l(\nu)\, PQ_l(\nu) \}$$

$$+ \lambda(\nu)\, P_n(\nu), \qquad n < L \qquad \text{(A9)}$$

The factor $\lambda(\nu)$ is defined from Eqn. (A9) with $g_o(\nu) = 1$, i.e.,

$$\lambda(\nu) = 1 - c\nu P \sum_{l=o}^{L} (2l+1)\, f_l\, g_l(\nu)\, Q_l(\nu)$$

when $\nu \notin (-1, 1)$, $\lambda(\nu) = 0$ and the asymptotic roots are obtained from the following transcendental eqn.

$$c\,\nu \sum_{l=o}^{L} (2l+1)\, f_l\, g_l(\nu)\, Q_l(\nu) = 1 \qquad \text{(A10)}$$

B. Modification of ν_L:

It has been shown in Chapter III, that the positivity of $K(\nu, \nu', b)$ is met if

$$\nu' \geq \frac{k_o^2 - \nu k_o \tan \frac{b+z_o}{k_o}}{\nu + k_o \tan \frac{b+z_o}{k_o}} \qquad \text{(B1)}$$

This condition is satisfied for all values of $\nu' \in \left(\frac{k_o}{\tan \frac{b+z_o}{k_o}}, 1\right)$ and $\nu \in (0, 1)$ as has been shown in

Chapter III. However, for the purpose of analysis, the lower limit of ν has also been changed to $\frac{k_o}{\tan \frac{b+z_o}{k_o}}$. This is obviously a conservative estimate. It will be shown here that if a new lower limit of ν and ν' is chosen as

$$\nu'_L = \frac{\nu_L}{2} = \frac{k_o}{2 \tan \frac{b+z_o}{k_o}}$$

the positivity criterion (B1) is still satisfied. The right hand side of (B1) has then a maximum value at $\nu = \nu_L/2$ which is equal to

$$\frac{k_o^2 - \frac{k_o}{2 \tan \frac{b+z_o}{k_o}} \cdot k_o \tan \frac{b+z_o}{k_o}}{\frac{k_o}{2 \tan \frac{b+z_o}{k_o}} + k_o \tan \frac{b+z_o}{k_o}} = \frac{k_o \tan \frac{b+z_o}{k_o}}{(1+ 2 \tan^2 \frac{b+z_o}{k_o})}$$

$$= \frac{k_o}{(2 \tan \frac{b+z_o}{k_o} + \cot \frac{b+z_o}{k_o})} < \nu'_L$$

Thus, it is found that the condition (B1) is met for all values of $\nu' \varepsilon (\nu'_L, 1)$. It is expected that this new lower limit $\nu'_L = \nu_L/2$ will induce a correction in critical thickness results. Further lowering of ν'_L may also be possible.

However, as no estimation of spectral radius for non-positive operators may be possible by existing theories, the positivity criterion has to be satisfied in any case.